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Computational Studies of Polynitroaromatic Molecules and the Development of Sensitivity Relationships

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13. ABSTRACT (Maximum 200 words) A computational study of 48 nitroaromatic molecules has been carried out with the objective of developing an understanding of how chemical structural features are related to the shock/impact sensitivities of these molecules. An <u>ab initio</u> self-consistent-field molecular orbital procedure was used to compute a variety of properties, including atomic charges, electrostatic potentials and ionization potentials. From the results of our computational analyses, it is suggested that the observed high sensitivities of hydroxytrinitroaromatics toward shock and impact may be due to the formation of small but significant quantities of unstable nitronic acid tautomers. When the hydroxynitroaromatics are excluded, the sensitivity is shown to be related to the C-NO ₂ linkage with the greatest instability, as measured by the electrostatic potential at the midpoint of the C-NO ₂ bond; this is an extension of a relationship discovered earlier. Hydrogen transfer and ring formation reactions of some alkyl- and amine-substituted nitroaromatics have been studied; the energetics of these reactions help to explain the differences in the thermal, shock and impact sensitivities of their larger trinitroaromatic analogues.				
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PREFACE

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TABLE OF CONTENTS

Section	Title	Page
I	INTRODUCTION	1
II	DISCUSSION.....	5
III	CONCLUDING REMARKS	18
APPENDIX	19
A	2,4,6-Trinitro- <u>m</u> -xylene.....	26
B	2,4,6-Trinitromesitylene.....	30
C	2,4,6-Trinitroethylbenzene.....	35
D	3-Chloro-2,4,6-trinitrotoluene	40
E	3-Bromo-2,4,6-trinitrotoluene	45
F	Ethyl(2,4,6-trinitrophenyl)carbamate.....	50
G	3-Amino-2,4,6-trinitrotoluene.....	55
H	3,5-Diamino-2,4,6-trinitrotoluene	60
I	<u>N</u> -Carboethoxy-2,4,6-trinitro- <u>m</u> -toluidine.....	65
J	3,5-Dibromo-2,4,6-trinitrotoluene.....	70
K	Ethyl picryl sulfide.....	75
L	1,3-Dimethoxy-2,4,6-trinitrobenzene	80
M	1,3-Dichloro-2,4,6-trinitrobenzene	85
N	Methyl 2,4,6-trinitrobenzoate.....	89
O	3-Chloro-2,4,6-trinitroanisole.....	94
P	Styphnic acid	99
Q	3-Amino-2,4,6-trinitroanisole	103
R	2,4,6-Trinitrophenylethanol.....	108
S	3,5-Dichloro-2,4,6-trinitroanisole.....	113
T	3,5-Diamino-2,4,6-trinitrophenol.....	118
U	2,4,6-Trinitrophloroglucinol.....	122
V	Aminopicric acid	126
W	2,3,4,6-Tetranitroaniline	131
X	1,3,5-Triamino-2,4,6-trinitrobenzene	135
Y	1,3-Diamino-2,4,6-trinitrobenzene.....	139
Z	2,4,6-Trinitrobenzyl alcohol.....	143
AA	2,4,6-Trinitrobenzonitrile	148

TABLE OF CONTENTS (Concluded)

Section	Title	Page
BB.	2,4,6-Trinitroacetophenone.....	153
CC.	3-Amino-2,4,6-trinitroethylbenzene	158
DD.	3-(Methylamino)-2,4,6-trinitrotoluene	163
EE.	<u>N,N</u> -Dimethylpicramide	168
FF.	<u>N</u> -Methylpicramide	173
GG.	3-Trifluoromethyl-2,4,6-trinitroaniline.....	178
HH.	1,3,5-Tribromo-2,4,6-trinitrobenzene.....	183
II.	2,4-Dibromo-1,3,5-trinitrobenzene.....	188
JJ.	3-Trifluoromethyl-2,4,6-trinitrophenol	193
KK.	<u>N</u> -Ethylpicramide.....	198
LL.	3-Hydroxy-2,4,6-trinitrotoluene	203
MM.	3,5-Dimethyl-2,4,6-trinitroanisole.....	208
NN.	2,4,6-Trinitro-3,5-dihydroxyaniline.....	213
OO.	1-Hydroxy-3-isopropyl-2,4,6-trinitrobenzene	218
PP.	3-Bromo-2,4,6-trinitroaniline	223
QQ.	2,3,4,5-Tetranitrotoluene.....	228
RR.	2,3,5,6-Tetranitrotoluene	233
SS.	2,3,4,6-Tetranitrotoluene	238
TT.	3-Bromopicric acid	243
UU.	3-Bromo-2,4,6-trinitroanisole	248
VV.	2,4,6-Trinitro-3-hydroxybenzoic acid	253
REFERENCES	258

LIST OF FIGURES

Figure	Title	Page
1	Plot of AFATL impact sensitivities versus those obtained from reference 23, measured in drop height in cm, for twelve nitroaromatics.....	9
2	Plot of AFATL impact sensitivities versus those obtained from reference 23, measured in drop height in cm, for six nitroaromatics.....	10
3	Correlation between impact sensitivity, as measured by impact drop height in cm (23), and $V_{mid,max}$ for eighteen nitroaromatics.....	16
A-1	Calculated electrostatic potential of 2,4,6-trinitro- <u>m</u> -xylene, in the plane 1.75 Å above the aromatic ring.....	29
B-1	Calculated electrostatic potential of 2,4,6-trinitromesitylene, in the plane 1.75Å above the N8 nitro group	33
B-2	Calculated electrostatic potential of 2,4,6-trinitromesitylene, in the plane 1.75Å above the N12 nitro group.....	34
C-1	Calculated electrostatic potential of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N10 nitro group.....	38
C-2	Calculated electrostatic potential of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group.....	39
D-1	Calculated electrostatic potential of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group	43
D-2	Calculated electrostatic potential of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group	44
E-1	Calculated electrostatic potential of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group.....	48
E-2	Calculated electrostatic potential of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group	49
F-1	Calculated electrostatic potential of ethyl(2,4,6-trinitrophenyl)-carbamate, in the plane 1.75Å above the N12 nitro group	53
F-2	Calculated electrostatic potential of ethyl(2,4,6-trinitrophenyl)-carbamate, in the plane 1.75Å above the N13 nitro group	54
G-1	Calculated electrostatic potential of 3-amino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group	58

LIST OF FIGURES (Continued)

Figure	Title	Page
H-1	Calculated electrostatic potential of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group	63
H-2	Calculated electrostatic potential of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group	64
I-1	Calculated electrostatic potential of <u>N</u> -carboethoxy-2,4,6-trinitro- <u>m</u> -toluidine, in the plane 1.75Å above the N30 nitro group.....	68
I-2	Calculated electrostatic potential of <u>N</u> -carboethoxy-2,4,6-trinitro- <u>m</u> -toluidine, in the plane 1.75Å above the N26 nitro group	69
J-1	Calculated electrostatic potential of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group	73
J-2	Calculated electrostatic potential of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group.....	74
K-1	Calculated electrostatic potential of ethyl picryl sulfide, in the plane 1.75Å above the N7 nitro group.....	78
K-2	Calculated electrostatic potential of ethyl picryl sulfide, in the plane 1.75Å above the N8 nitro group	79
L-1	Calculated electrostatic potential of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75Å above the N7 nitro group.....	83
L-2	Calculated electrostatic potential of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75Å above the N11 nitro group	84
M-1	Calculated electrostatic potential of 1,3-dichloro-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring	88
N-1	Calculated electrostatic potential of methyl 2,4,6-trinitrobenzoate, in the plane 1.75Å above the N10 nitro group.....	92
N-2	Calculated electrostatic potential of methyl 2,4,6-trinitrobenzoate, in the plane 1.75Å above the N9 nitro group	93
O-1	Calculated electrostatic potential of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group	97
O-2	Calculated electrostatic potential of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group.....	98

LIST OF FIGURES (Continued)

Figure	Title	Page
P-1	Calculated electrostatic potential of styphnic acid, in the plane 1.75 Å above the aromatic ring	102
Q-1	Calculated electrostatic potential of 3-amino-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group	106
Q-2	Calculated electrostatic potential of 3-amino-2,4,6-trinitroanisole, in the plane 1.75Å above the N9 nitro group	107
R-1	Calculated electrostatic potential of 2,4,6-trinitrophenylethanol, in the plane 1.75Å above the N8 nitro group	111
R-2	Calculated electrostatic potential of 2,4,6-trinitrophenylethanol, in the plane 1.75Å above the N12 nitro group	112
S-1	Calculated electrostatic potential of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group.....	116
S-2	Calculated electrostatic potential of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N9 nitro group	117
T-1	Calculated electrostatic potential of 3,5-diamino-2,4,6-trinitrophenol, in the plane 1.75 Å above the aromatic ring.....	121
U-1	Calculated electrostatic potential of 2,4,6-trinitrophenylglucitol, in the plane 1.75Å above the N18 nitro group	125
V-1	Calculated electrostatic potential of aminopicric acid, in the plane 1.75Å above the N10 nitro group	129
V-2	Calculated electrostatic potential of aminopicric acid, in the plane 1.75Å above the N9 nitro group	130
W-1	Calculated electrostatic potential of 2,3,4,6-tetranitroaniline, in the plane 1.75 Å above the aromatic ring	134
X-1	Calculated electrostatic potential of 1,3,5-triamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring.....	138
Y-1	Calculated electrostatic potential of 1,3-diamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring.....	142
Z-1	Calculated electrostatic potential of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N8 nitro group	146

LIST OF FIGURES (Continued)

Figure	Title	Page
Z-2	Calculated electrostatic potential of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N12 nitro group.....	147
AA-1	Calculated electrostatic potential of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N10 nitro group.....	151
AA-2	Calculated electrostatic potential of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N9 nitro group	152
BB-1	Calculated electrostatic potential of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N9 nitro group	156
BB-2	Calculated electrostatic potential of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N7 nitro group	157
CC-1	Calculated electrostatic potential, of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group	161
CC-2	Calculated electrostatic potential of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N12 nitro group	162
DD-1	Calculated electrostatic potential of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group.....	166
DD-2	Calculated electrostatic potential of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group.....	167
EE-1	Calculated electrostatic potential of <u>N,N</u> -dimethylpicramide, in the plane 1.75Å above the N9 nitro group	171
EE-2	Calculated electrostatic potential of <u>N,N</u> -dimethylpicramide, in the plane 1.75Å above the N8 nitro group	172
FF-1	Calculated electrostatic potential of <u>N</u> -methylpicramide, in the plane 1.75Å above the N9 nitro group.....	176
FF-2	Calculated electrostatic potential of <u>N</u> -methylpicramide, in the plane 1.75Å above the N8 nitro group	177
GG-1	Calculated electrostatic potential of 3-trifluoromethyl-2,4,6-trinitroaniline, in the plane 1.75Å above the N11 nitro group	181
GG-2	Calculated electrostatic potential of 3-trifluoromethyl-2,4,-trinitroaniline, in the plane 1.75Å above the N10 nitro group	182

LIST OF FIGURES (Continued)

Figure	Title	Page
HH-1	Calculated electrostatic potential of 1,3,5-tribromo-2,4,6-trinitro- benzene, in the plane 1.75Å above the N7 nitro group.....	186
HH-2	Calculated electrostatic potential of 1,3,5-tribromo-2,4,6-trinitro- benzene, in the plane 1.75Å above the N8 nitro group	187
II-1	Calculated electrostatic potential of 2,4-dibromo-1,3,5-trinitro- benzene, in the plane 1.75Å above the N9 nitro group.....	191
II-2	Calculated electrostatic potential of 2,4-dibromo-1,3,5-trinitro- benzene, in the plane 1.75Å above the N7 nitro group.....	192
JJ-1	Calculated electrostatic potential of 3-trifluoromethyl-2,4,6-trinitro- phenol, in the plane 1.75Å above the N9 nitro group	196
JJ-2	Calculated electrostatic potential of 3-trifluoromethyl-2,4,6-trinitro- phenol, in the plane 1.75Å above the N10 nitro group.....	197
KK-1	Calculated electrostatic potential of <u>N</u> -ethylpicramide, in the plane 1.75Å above the N7 nitro group	201
KK-2	Calculated electrostatic potential of <u>N</u> -ethylpicramide, in the plane 1.75Å above the N8 nitro group	202
LL-1	Calculated electrostatic potential of 3-hydroxy-2,4,6-trinitro- toluene, in the plane 1.75Å above the N9 nitro group.....	206
LL-2	Calculated electrostatic potential of 3-hydroxy-2,4,6-trinitro- toluene, in the plane 1.75Å above the N10 nitro group	207
MM-1	Calculated electrostatic potential of 3,5-dimethyl-2,4,6-trinitro- anisole, in the plane 1.75Å above the N10 nitro group.....	211
MM-2	Calculated electrostatic potential of 3,5-dimethyl-2,4,6-trinitro- anisole, in the plane 1.75Å above the N12 nitro group.....	212
NN-1	Calculated electrostatic potential of 2,4,6-trinitro-3,5-dihydroxy- aniline, in the plane 1.75Å above the N7 nitro group.....	216
NN-2	Calculated electrostatic potential of 2,4,6-trinitro-3,5-dihydroxy- aniline, in the plane 1.75Å above the N8 nitro group	217
OO-1	Calculated electrostatic potential of 1-hydroxy-3-isopropyl-2,4,6- trinitrobenzene, in the plane 1.75Å above the N8 nitro group.....	221

LIST OF FIGURES (Concluded)

Figure	Title	Page
OO-2	Calculated electrostatic potential of 1-hydroxy-3-isopropyl-2,4,6-trinitrobenzene, in the plane 1.75Å above the N9 nitro group.....	222
PP-1	Calculated electrostatic potential of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N7 nitro group.....	226
PP-2	Calculated electrostatic potential of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N10 nitro group.....	227
QQ-1	Calculated electrostatic potential of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group	231
QQ-2	Calculated electrostatic potential of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group	232
RR-1	Calculated electrostatic potential of 2,3,5,6-tetranitrotoluene, in the plane 1.75Å above the N8 nitro group.....	236
RR-2	Calculated electrostatic potential of 2,3,5,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group	237
SS-1	Calculated electrostatic potential of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group	241
SS-2	Calculated electrostatic potential of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group.....	242
TT-1	Calculated electrostatic potential of 3-bromopicric acid, in the plane 1.75Å above the N10 nitro group.....	246
TT-2	Calculated electrostatic potential of 3-bromopicric acid, in the plane 1.75Å above the N11 nitro group.....	247
UU-1	Calculated electrostatic potential of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group.....	251
UU-2	Calculated electrostatic potential of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group.....	252
VV-1	Calculated electrostatic potential of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N8 nitro group.....	256
VV-2	Calculated electrostatic potential of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N10 nitro group	257

LIST OF TABLES

Table	Title	Page
1.	Computed and Experimental Properties of Sixty Nitroaromatics.....	4
2.	Properties of Some Nitroaromatics.....	11
3.	Calculated 3-21G Energies.....	20
4.	Calculated STO-3G energies of <i>o</i> -nitrocumene and related systems.....	23

SECTION I

INTRODUCTION

The objective of this project has been to carry out computational studies of certain nitro-aromatic molecules in order to develop an understanding of how the sensitivities of these molecules toward shock and impact are related to their chemical structures. This knowledge could then be used to design molecules with desired sensitivity and explosive performance characteristics.

We have investigated 48 substituted trinitroaromatic molecules. All of the molecules examined had been selected for this purpose by the Air Force Armament Laboratory (AFATL). They are listed below, together with the source of each one's crystallographically determined structure (References 1-12).

- A. 2,4,6-Trinitro-m-xylene (Reference 1)
- B. 2,4,6-Trinitromesitylene (Reference 2)
- C. 2,4,6-Trinitroethylbenzene (Reference 3)
- D. 3-Chloro-2,4,6-trinitrotoluene (Reference 3)
- E. 3-Bromo-2,4,6-trinitrotoluene (Reference 3)
- F. Ethyl(2,4,6-trinitrophenyl)carbamate (Reference 4)
- G. 3-Amino-2,4,6-trinitrotoluene (Reference 4)
- H. 3,5-Diamino-2,4,6-trinitrotoluene (Reference 4)
- I. N-Carboethoxy-2,4,6-trinitro-m-toluidine (Reference 2)
- J. 3,5-Dibromo-2,4,6-trinitrotoluene (Reference 3)
- K. Ethyl picryl sulfide (Reference 3)
- L. 1,3-Dimethoxy-2,4,6-trinitrobenzene (Reference 2)
- M. 1,3-Dichloro-2,4,6-trinitrobenzene (Reference 5)
- N. Methyl 2,4,6-trinitrobenzoate (Reference 2)
- O. 3-Chloro-2,4,6-trinitroanisole (Reference 6)
- P. Styphnic acid (Reference 7)
- Q. 3-Amino-2,4,6-trinitroanisole (Reference 4)
- R. 2,4,6-Trinitrophenylethanol (Reference 2)

- S. 3,5-Dichloro-2,4,6-trinitroanisole (Reference 2)
- T. 3,5-Diamino-2,4,6-trinitrophenol (Reference 8)
- U. 2,4,6-Trinitrophloroglucinol (Reference 7)
- V. Aminopicric acid (Reference 9)
- W. 2,3,4,6-Tetranitroaniline (Reference 10)
- X. 1,3,5-Triamino-2,4,6-trinitrobenzene (Reference 11)
- Y. 1,3-Diamino-2,4,6-trinitrobenzene (Reference 12)
- Z. 2,4,6-Trinitrobenzyl alcohol (Reference 2)
- AA. 2,4,6-Trinitrobenzonitrile (Reference 2)
- BB. 2,4,6-Trinitroacetophenone (Reference 2)
- CC. 3-Amino-2,4,6-trinitroethylbenzene (Reference 3)
- DD. 3-(Methylamino)-2,4,6-trinitrotoluene (Reference 3)
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- FF. N-Methylpicramide (Reference 3)
- GG. 3-Trifluoromethyl-2,4,6-trinitroaniline (Reference 2)
- HH. 1,3,5-Tribromo-2,4,6-trinitrobenzene (Reference 3)
- II. 2,4-Dibromo-1,3,5-trinitrobenzene (Reference 3)
- JJ. 3-Trifluoromethyl-2,4,6-trinitrophenol (Reference 6)
- KK. N-Ethylpicramide (Reference 6)
- LL. 3-Hydroxy-2,4,6-trinitrotoluene (Reference 6)
- MM. 3,5-Dimethyl-2,4,6-trinitroanisole (Reference 6)
- NN. 2,4,6-Trinitro-3,5-dihydroxyaniline (Reference 6)
- OO. 1-Hydroxy-3-isopropyl-2,4,6-trinitrobenzene (Reference 6)
- PP. 3-Bromo-2,4,6-trinitroaniline (Reference 6)
- QQ. 2,3,4,5-Tetranitrotoluene (Reference 6)
- RR. 2,3,5,6-Tetranitrotoluene (Reference 6)
- SS. 2,3,4,6-Tetranitrotoluene (Reference 6)

TT. 3-Bromopicric acid (Reference 6)

UU. 3-Bromo-2,4,6-trinitroanisole (Reference 6)

VV. 2,4,6-Trinitro-3-hydroxybenzoic acid (Reference 6)

In the selected substituted trinitroaromatics, the mean plane of each nitro group is generally inclined from the mean plane of the benzene ring by either twisting around the C-N bond or simply bending at the attached carbon atom, or both. The angles of rotation for the nitro groups range from near 0 degrees (coplanar with the benzene ring) to essentially 90 degrees. All of the molecules (except TATB) exhibit some rotation of the nitro groups.

Assuming the van der Waals radii of the O and the H atoms are 1.40 and 1.20 angstroms respectively, the H...O distances between nonbonding atoms which are less than 2.50 angstroms strongly indicate hydrogen bonding. All of the substituted trinitrobenzenes are observed to have some hydrogen bonding.

In Table 1 is given a compilation of some computed and experimental properties for the forty-eight nitroaromatics included in this contract plus the twelve studied in an earlier one-year contract AFATL-88-107. In addition, the following data are presented in Appendices for each of the forty-eight molecules included in this contract:

- (a) Z-matrix. This is the format of the input for the GAUSSIAN programs, which we use for our computational analyses. This includes selected bond distances, angles and dihedral angles.
- (b) Total molecular energy, in hartrees.
- (c) Ionization potential, approximated as the calculated energy of the highest occupied molecular orbital.
- (d) Atomic charges, calculated by means of Mulliken's population analysis procedure.
- (e) Calculated dipole moment, in Debyes.
- (f) Electrostatic potentials, V_{mid} , at the midpoints of the C-NO₂ bonds, as approximated by the formula: $V_{\text{mid}} = Q_{\text{C}}/0.5R + Q_{\text{N}}/0.5R$. Q_{C} and Q_{N} are the charges on the carbon and nitrogen; R is the C-N bond length, in bohrs (1 bohr = 0.55292 Å).
- (g) Bond orders of C-NO₂ and N-O bonds, calculated using the formula:

$$\text{Bond Order} = \frac{11.92}{R^3 v^2} \quad (1)$$

R is the actual bond length in Angstroms, and v is a parameter that is characteristic of given bond types and can be regarded as representing an effective length of the bond. This formula is a modification of our earlier bond order expression (Reference 13) which involved the

TABLE 1. COMPUTED AND EXPERIMENTAL
PROPERTIES OF SIXTY NITROAROMATICS^a

Molecule	V _{mid,max}	IP (eV)	Dipole	Impact Drop Height ^b	
			Moment (Debye)	(cm) Reference 32	AFATL
2,4,6-Trinitroanisole	0.187	8.44	2.12	192	79.3 ^c
α,α,α -Trifluoro-2,4,6-trinitro- toluene	0.237	8.88	0.81	n.a.	101.7 ^c
2,4,6-Trinitrophenylhydrazine	0.193	8.13	4.37	n.a.	21.9
2,4,6-Trinitrophenetole	0.258	8.52	2.10	190	n.a.
2,4,6-Trinitrobenzamide	0.206	8.71	2.52	n.a.	62.8 ^c
2,4,6-Trinitrobenzoic Acid	0.205	8.79	1.15	109	91.4
2,4,6-Trinitrobenzaldehyde	0.217	8.83	1.24	36	53.5
1,3,5-Trinitro-2-n-propyl- benzene	0.204	8.48	1.73	n.a.	48.1 ^c
meta-Dinitrobenzene	0.182	8.15	2.97 (4.10)	n.a.	n.a.
2,4,6-Trinitrochlorobenzene	0.234	8.80	0.85	79	72.5 ^c
2,4,6-Trinitrotoluene	0.209	8.57	1.17 (1.37)	160	105.4, 61.7 ^c
1,3,5-Trinitrobenzene	0.208	8.71	0.26 (0.00)	100	49.8
2,4,6-Trinitroaniline	0.174	8.24	2.31	177	137.8 ^c
2,4,6-Trinitrophenol	0.203	8.40	2.76	87	44.7
2,4,6-Trinitrobenzylchloride	0.214	8.74	1.53	44	79.3
2,4,6-Trinitro- <i>m</i> -xylene	0.204	8.52	1.27	n.a.	75.0
2,4,6-Trinitromesitylene	0.189	8.52	0.11	n.a.	52.6
2,4,6-Trinitroethylbenzene	0.203	8.59	1.13	n.a.	n.a.
3-Chloro-2,4,6-trinitrotoluene	0.205	8.43	2.41	n.a.	79.5
3-Bromo-2,4,6-trinitrotoluene	0.200	8.61	1.25	n.a.	94.7
Ethyl(2,4,6-trinitrophenyl)- carbamate	0.206	8.37	2.92	n.a.	n.a.
3-Amino-2,4,6-trinitrotoluene	0.169	8.23	2.09	n.a.	123.8 ^c
3,5-Diamino-2,4,6-trinitro- toluene	0.132	7.82	1.47	n.a.	n.a.
<i>N</i> -Carboethoxy-2,4,6-trinitro- <i>m</i> -toluidine	0.198	8.36	2.51	n.a.	n.a.
3,5-Dibromo-2,4,6-trinitro- toluene	0.209	8.83	1.26	n.a.	n.a.
Ethyl picryl sulfide	0.185	7.91	2.13	n.a.	n.a.

TABLE 1. COMPUTED AND EXPERIMENTAL PROPERTIES
OF SIXTY NITROAROMATICS (Continued)^a

Molecule	V _{mid,max}	IP (eV)	Dipole	Impact Drop Height ^b	
			Moment (Debye)	(cm) Reference 32	AFATL
1,3-Dimethoxy-2,4,6-trinitro- benzene	0.185	8.66	2.46	251	44.0
1,3-Dichloro-2,4,6-trinitro- benzene	0.219	8.90	1.10	n.a.	85.1
Methyl 2,4,6-trinitrobenzoate	0.223	8.78	1.28	90	93.1 ^c
3-Chloro-2,4,6-trinitroanisole	0.202	8.73	2.54	n.a.	151.6
Styphnic acid	0.170	8.10	1.78	43	24.0
3-Amino-2,4,6-trinitroanisole	0.165	8.36	2.19	>325	164.7 ^c
2,4,6-Trinitrophenylethanol	0.210	8.22	2.67	68	96.4
3,5-Dichloro-2,4,6-trinitro- anisole	0.202	8.81	2.89	75	94.7
3,5-Diamino-2,4,6-trinitro- phenol	0.125	7.95	2.87	112	n.a.
2,4,6-Trinitrophenylglucitol	0.143	7.86	2.94	27	n.a.
Aminopicric acid	0.151	8.31	0.69	138	n.a.
2,3,4,6-Tetranitroaniline	0.236	8.49	4.85	41	27.7
1,3,5-Triamino-2,4,6-trinitro- benzene	0.105	7.88	0.78	>325	n.a.
1,3-Diamino-2,4,6-trinitro- benzene	0.146	8.09	1.48	320	150.7 ^c
2,4,6-Trinitrobenzyl alcohol	0.217	8.50	2.06	52	57.5
2,4,6-Trinitrobenzonitrile	0.213	8.95	2.36	140	72.1
2,4,6-Trinitroacetophenone	0.210	8.66	1.83	79	117.4 ^c
3-Amino-2,4,6-trinitroethyl- benzene	0.176	8.20	2.23	n.a.	n.a.
3-(Methylamino)-2,4,6-trinitro- toluene	0.172	7.95	2.82	n.a.	n.a.
<u>N,N</u> -Dimethylpicramide	0.193	8.03	3.63	n.a.	66.7 ^c
<u>N</u> -Methylpicramide	0.185	8.08	3.71	n.a.	82.1
3-Trifluoromethyl-2,4,6- trinitroaniline	0.184	8.47	2.99	n.a.	101.7
1,3,5-Tribromo-2,4,6-trinitro- benzene	0.201	8.99	0.03	n.a.	n.a.

TABLE 1. COMPUTED AND EXPERIMENTAL PROPERTIES
OF SIXTY NITROAROMATICS (Concluded)^a

Molecule	V _{mid,max}	IP (eV)	Dipole	Impact Drop Height ^b	
			Moment (Debye)	(cm) Reference 32	AFATL
2,4-Dibromo-1,3,5-trinitro- benzene	0.213	8.82	0.27	n.a.	n.a.
3-Trifluoromethyl-2,4,6- trinitrophenol	0.195	8.58	2.25	n.a.	121.6 ^c
N-Ethylpicramide	0.176	8.01	3.80	n.a.	60.6 ^c
3-Hydroxy-2,4,6-trinitro- toluene	0.174	8.26	0.72	191	73.8
3,5-Dimethyl-2,4,6-trinitro- anisole	0.190	8.34	1.34	n.a.	47.0 ^c
2,4,6-Trinitro-3,5-dihydroxy- aniline	0.142	7.69	4.40	32	27.8
1-Hydroxy-3-isopropyl-2,4,6- trinitrobenzene	0.182	8.39	0.83	n.a.	96.4
3-Bromo-2,4,6-trinitroaniline	0.183	8.49	1.69	n.a.	n.a.
2,3,4,5-Tetranitrotoluene	0.220	8.83	6.19	n.a.	n.a.
2,3,5,6-Tetranitrotoluene	0.225	8.88	0.93	n.a.	n.a.
2,3,4,6-Tetranitrotoluene	0.223	8.91	3.54	n.a.	n.a.
3-Bromopicric acid	0.185	8.54	1.66	n.a.	n.a.
3-Bromo-2,4,6-trinitroanisole	0.196	8.69	1.79	n.a.	n.a.
2,4,6-Trinitro-3-hydroxy- benzoic acid	0.189	8.48	1.24	n.a.	n.a.

^aExperimental values for ionization potentials and dipole moments, when available, are given in parentheses.

^bThe impact drop heights were measured with 2.5 kg weights except for those designated with a superscript c. n. a. stands for not available.

^cData were measured with 5.0 kg weights.

force constant and the bond length; it was introduced in order to avoid the time and space-consuming computations required to calculate force constants. We have shown that by choosing appropriate values for v , very good agreement can be obtained with the results of the original formula.

- (h) Plots showing calculated molecular electrostatic potential in various planes. This potential is obtained using the exact formula:

$$V(\mathbf{r}) = \sum_A \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}') d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|} \quad (2)$$

Z_A is the charge on nucleus A, located at \mathbf{R}_A , and $\rho(\mathbf{r})$ is the electronic density function, obtained from the computed molecular wave function. The dashed contours represent negative potentials and the solid contours correspond to the zero and positive contours. The zero contour is marked.

SECTION II DISCUSSION

In the area of nitroaromatics, a number of studies have been carried out which support the idea that C-NO₂ bonds are of key importance in determining impact and shock sensitivities (References 14-19). Some time ago we found a correlation between the shock/impact sensitivities of a group of six nitroaromatics and the quantity V_{mid} , the electrostatic potential at the midpoint of the longest C-NO₂ bond in each system (Reference 17). V_{mid} is approximated from calculated atomic charges, as given in equation (3).

$$V_{\text{mid}} = \frac{Q_{\text{C}}}{0.5 R} + \frac{Q_{\text{N}}}{0.5 R} \quad (3)$$

Q_{C} and Q_{N} are the charges on the carbon and nitrogen, obtained from the Mulliken population analysis (Reference 20) of the molecular orbital wave function; R is the C-N bond length in Å. V_{mid} is almost invariably positive for nitroaromatic C-NO₂ bonds, as a consequence of the calculated charges of the carbon and nitrogen atom forming these bonds usually both being positive. This suggests that the magnitude of V_{mid} reflects a certain degree of instability in these bonds, an interpretation that is supported by Fliszar's formulation of bond energy in terms of atomic charges and the reciprocal of the bond length (References 21 and 22).

During the course of this project we have computed V_{mid} for the C-NO₂ bonds of a large number of nitroaromatics. Table 2 lists the largest value, $V_{\text{mid,max}}$, for each of a group of 26 nitroaromatics, along with its measured impact drop height value. It should be noted that a serious problem encountered in seeking to understand and interpret experimentally-determined sensitivity data is the very marked degree to which these depend upon the laboratory at which the measurements were made. This can be seen in Figures 1 and 2, which show the absence of any correlation between impact sensitivities obtained at AFATL and those given in Reference 32. (If the point for 1,3-dimethoxy-2,4,6-trinitrobenzene were removed from Figure 1, the linear correlation coefficient would increase to 0.53, which is a marked improvement but still very poor.)

It is seen in Table 2 that trinitroaromatics with substituents that are strong resonance donors, such as -NH₂, -OH, -OCH₃ and -OC₂H₅, have $V_{\text{mid,max}}$ values that are less than that of 1,3,5-trinitrobenzene (I), which can be viewed as a reference molecule (since it has only hydrogens as non-nitro substituents). This is consistent with these groups having a strengthening effect on

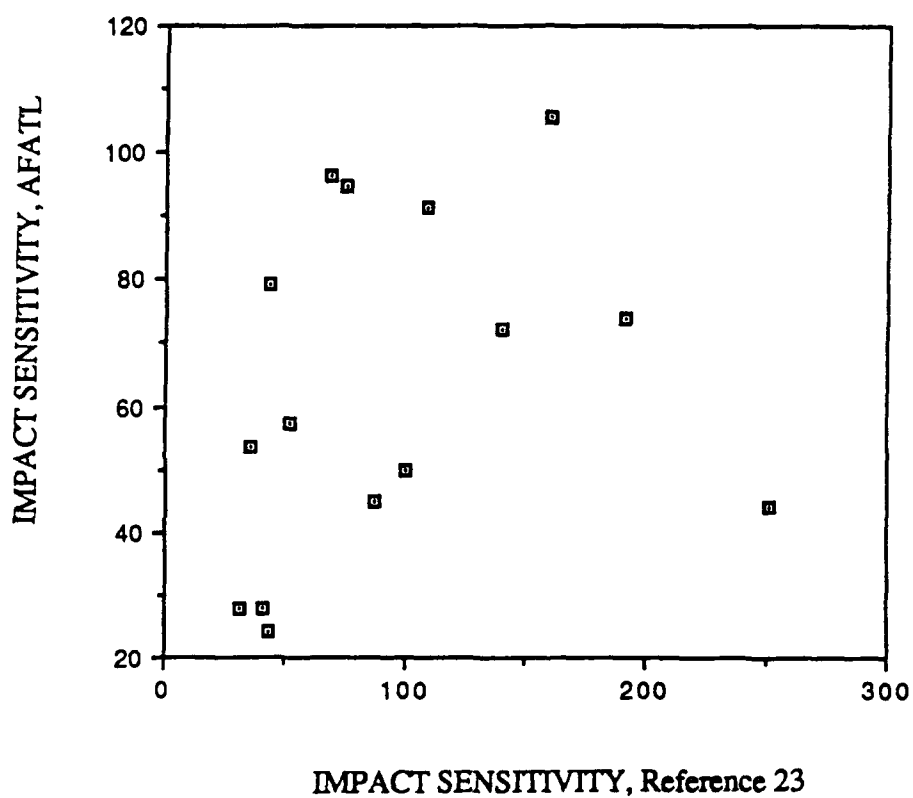


Figure 1. Plot of AFATL impact sensitivities versus those obtained from Reference 32, measured in drop height in cm, for fifteen nitroaromatics. Both sets of data were measured with 2.5 kg weights. The linear correlation coefficient is 0.26.

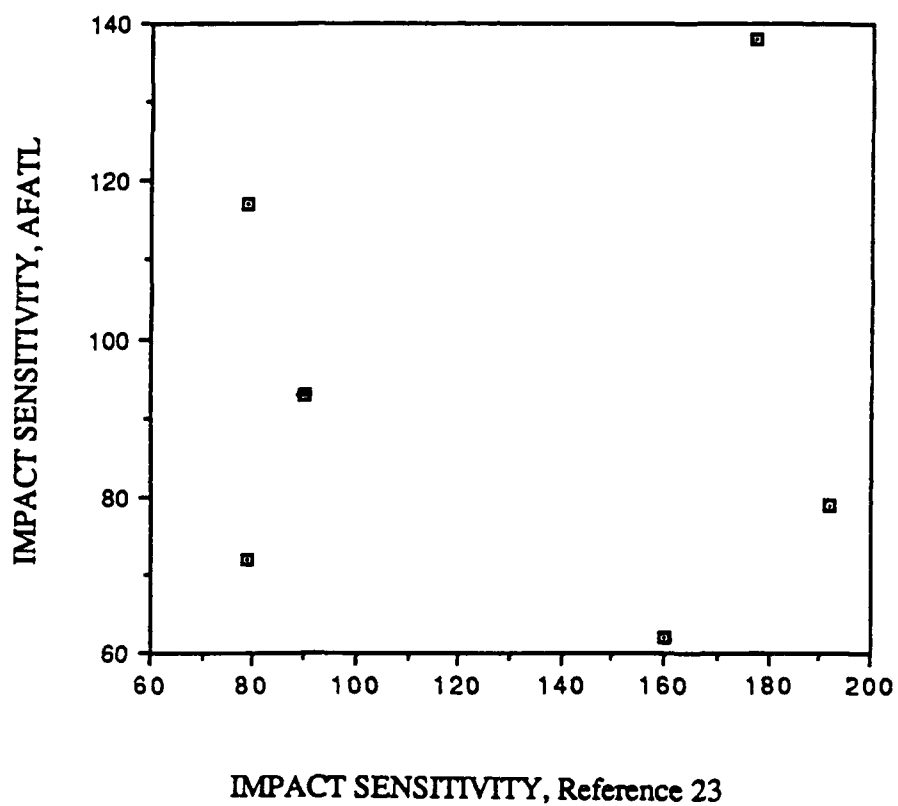


Figure 2. Plot of AFATL impact sensitivities versus those obtained from Reference 32, measured in drop height in cm, for six nitroaromatics. The Navy data were measured using 2.5 kg weights; the AFATL data were obtained with 5.0 kg weights. The linear correlation coefficient is 0.02.

TABLE 2. PROPERTIES OF SOME NITROAROMATICS

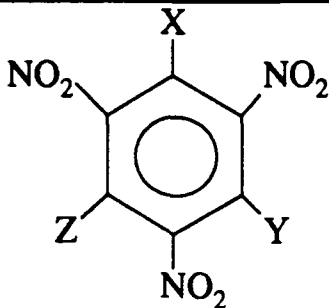
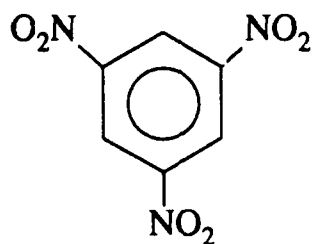
 XYZ	Impact Drop Height ^a (cm)	V _{mid,max}	$\left(\frac{1}{R}\right)_{\text{ave}}, \text{A}^{-1}$	Reference for Structure
OH, OH, OH	27	.143	.692	Reference 7
NH ₂ , OH, OH	32	.142	.698	Reference 23
CHO, H, H	36	.217	.675	Reference 23
NH ₂ , NO ₂ , H	41	.240	.683	Reference 10
OH, OH, H	43	.170	.685	Reference 7
CH ₂ Cl, H, H	44	.214	.675	Reference 7
CH ₂ OH, H, H	52	.217	.679	Reference 7
C ₂ H ₄ OH, H, H	68	.210	.678	Reference 7
OCH ₃ , Cl, Cl	75	.202	.677	Reference 7
Cl, H, H	79	.234	.672	Reference 24
COCH ₃ , H, H	79	.210	.678	Reference 7
OH, H, H	87	.203	.684	Reference 25
COOCH ₃ , H, H	90	.223	.680	Reference 7
H, H, H	100	.208	.675	Reference 26
COOH, H, H	109	.205	.675	Reference 27
OH, NH ₂ , NH ₂	112	.125	.699	Reference 8
OH, NH ₂ , H	138	.151	.688	Reference 27
CN, H, H	140	.213	.675	Reference 7
CH ₃ , H, H	160	.209	.678	Reference 28
NH ₂ , H, H	177	.174	.681	Reference 29
OC ₂ H ₅ , H, H	190	.198	.681	Reference 30
OCH ₃ , H, H	192	.187	.679	Reference 31
OCH ₃ , OCH ₃ , H	251	.185	.678	Reference 7
NH ₂ , NH ₂ , H	320	.146	.689	Reference 12
OCH ₃ , NH ₂ , H	>325	.165	.685	Reference 7
NH ₂ , NH ₂ , NH ₂	>325	.103	.705	Reference 11

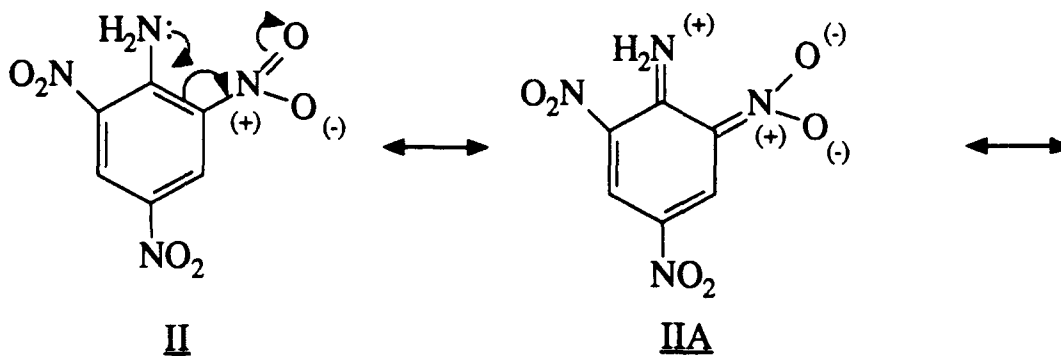
Table 2. Footnote:

- ^a Impact sensitivity is measured as the height from which a given weight must be dropped on a compound to produce detonation fifty percent of the time. Thus, the smaller the value given, the more sensitive is the compound toward impact. These data are taken from Reference 32.
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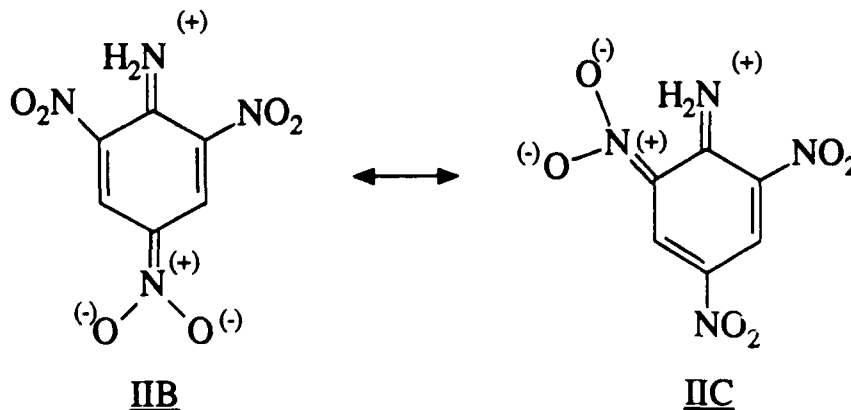


I

C-NO₂ bonds, as indicated by structures IIA - IIC and by the increase in $(1/R)_{ave}$ compared to 1,3,5-trinitrobenzene, I (see Table 2). All of these molecules also have lower $V_{mid,max}$ values than does I.

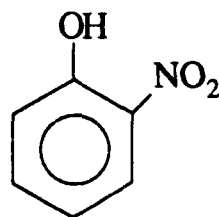


(4)

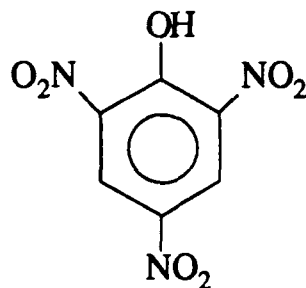


It has been noted earlier, for nitroaromatics, that a marked decrease in sensitivity accompanies an increase in the number of amine groups (References 16, 32 and 33). It is seen in Table 2 that alkoxy substituents and combinations of -NH₂ and -OR groups have similar effects upon impact sensitivities, as indicated by their large impact drop heights. However hydroxynitroaromatics are found to be very sensitive, despite the fact that -OH has resonance capabilities analogous to -NH₂ and -OR.

This observed sensitizing effect of the hydroxyl group in trinitroaromatics led us to investigate computationally the basis for this behavior, using *o*-nitrophenol (**III**) as a model for picric acid (**IV**) (Reference 34). The combined electron-withdrawing power of the three nitro groups in picric acid



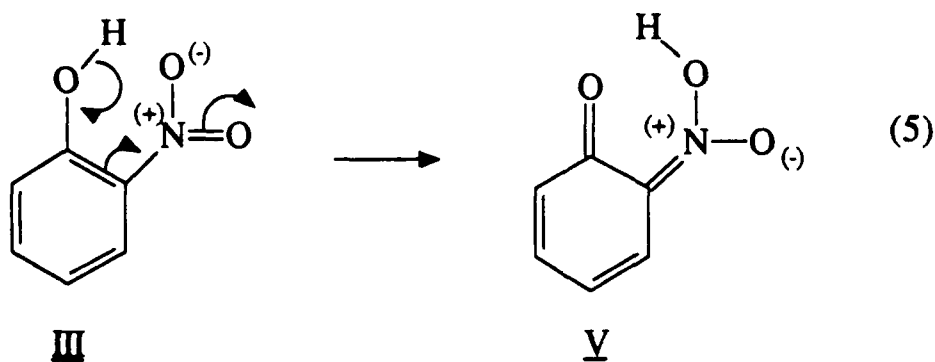
III



IV

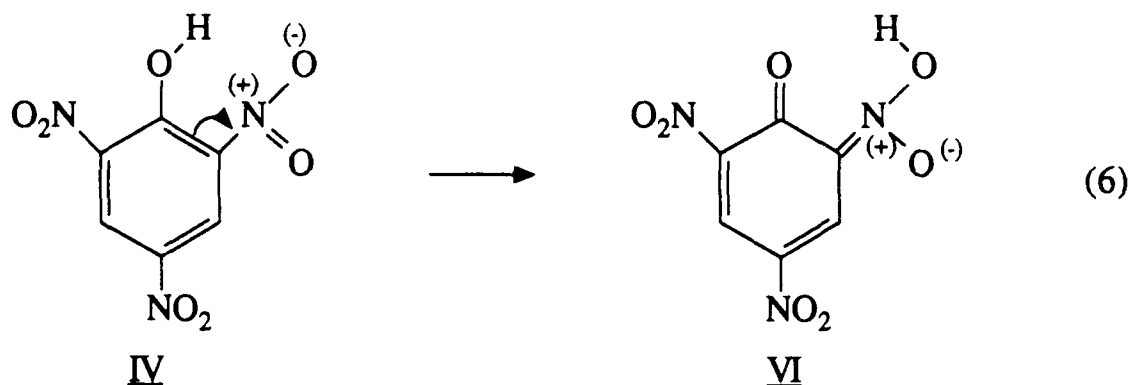
makes the hydroxyl hydrogen quite positive in nature. For example, whereas phenol is only weakly acidic, with a pK_a of 9.9, picric acid is a relatively strong acid; its pK_a of 0.38 is comparable to that of trichloroacetic acid (0.70) (Reference 35). In addition, the crystal structure of picric acid indicates significant hydrogen bonding between the hydroxyl and an ortho nitro group (Reference 25). The O...O separation is 2.55 Å, which is near the shorter end of the range that has been identified as typical of O-H...O hydrogen bonds (2.50 - 2.80 Å) (Reference 36). Our optimized 3-21G structure of **III** shows an O...O separation of 2.55 Å, the same as that found in the crystal structure of picric acid, and an OH...O distance of 1.75 Å (typical of a strong oxygen-hydrogen hydrogen bond (Reference 36)).

The labile nature of the hydroxyl hydrogen in **III** and its proximity to the nitro oxygen led us to investigate the possibility of hydrogen migration to the nitro oxygen, as shown in equation (5). **V** is a nitronic acid; the latter are known to be reactive, unstable systems (Reference 37). Thus, if a



process analogous to equation (5) were to occur for picric acid (**IV**), this would represent a decomposition mechanism that could account for its instability, and that of the dihydroxy and

trihydroxy derivatives of trinitrobenzene. At the 3-21G level, the nitronic acid V is 15.4 kcal/mole higher in energy than III. We suggest from these calculated results that the observed high sensitivity of hydroxytrinitroaromatics toward shock and impact may be due to some significant fraction of the molecules being in the form of an unstable nitronic acid, produced through a process



such as is shown in equation (6) for picric acid. The proton transfer shown in equation (6) could result, for example, from a vibrational excitation of the O-H bond brought about by the energy input associated with shock or impact. We have shown that there is no similar tendency for nitronic acid formation in aminonitroaromatics (References 34 and 38), revealing a major difference between the amino and hydroxynitroaromatics that may account in part for their contrasting sensitivities.

In light of the anomalous effect of -OH on sensitivity, we have excluded all hydroxytrinitroaromatics in seeking correlations between V_{mid} and impact sensitivity. Figure 3 shows measured impact drop heights plotted against $V_{\text{mid,max}}$ values for the molecules in Table 2 that have no hydroxyl groups. The calculated linear correlation coefficient is 0.86. It is noteworthy that nitroaromatics bearing α -CH linkages do not need to be treated separately, as was found to be necessary in establishing the OB₁₀₀ correlations with impact sensitivity (Reference 32). The present relationship suggests that the C-NO₂ linkage with the greatest instability, as indicated by $V_{\text{mid,max}}$, may be a key bond involved in initiating decomposition in nitroaromatics subjected to impact.

As part of our continuing study of the relationship between molecular properties and shock, impact and thermal sensitivity, we have investigated the possibilities of hydrogen transfer reactions, analogous to those shown in equations (5) and (6) for *o*-nitrophenol and picric acid, for the model systems *o*-nitroaniline (VII), *o*-nitrotoluene (VIII) and *o*-nitrocumene (IX). VII - IX are

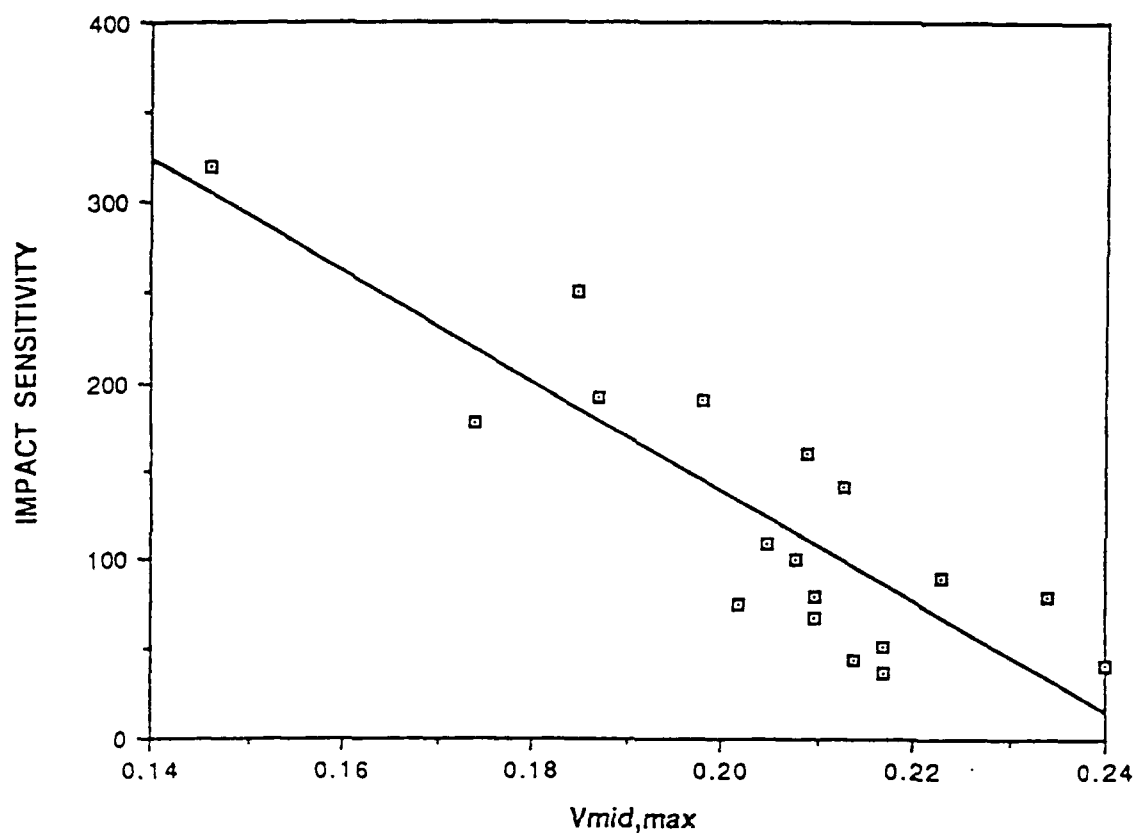
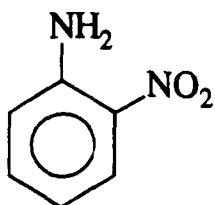
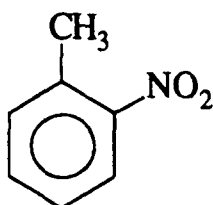


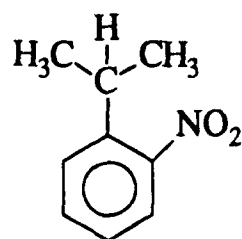
Figure 3. Correlation between impact sensitivity, as measured by impact drop height in cm (Reference 32), and $V_{mid,max}$ for eighteen nitroaromatics. Data are taken from Table 2, excluding hydroxynitroaromatics and molecules for which the impact sensitivities are given as greater than 325 cm. The least squares equation of the line is $y = 755.01 - 3084.27x$, with a correlation coefficient of 0.86.



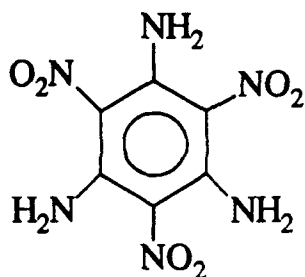
VII



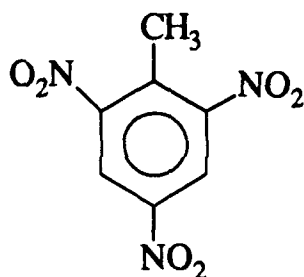
VIII



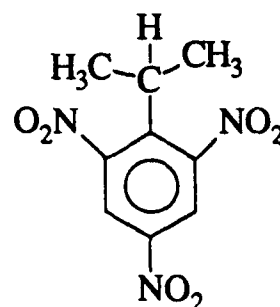
IX



X, TATB



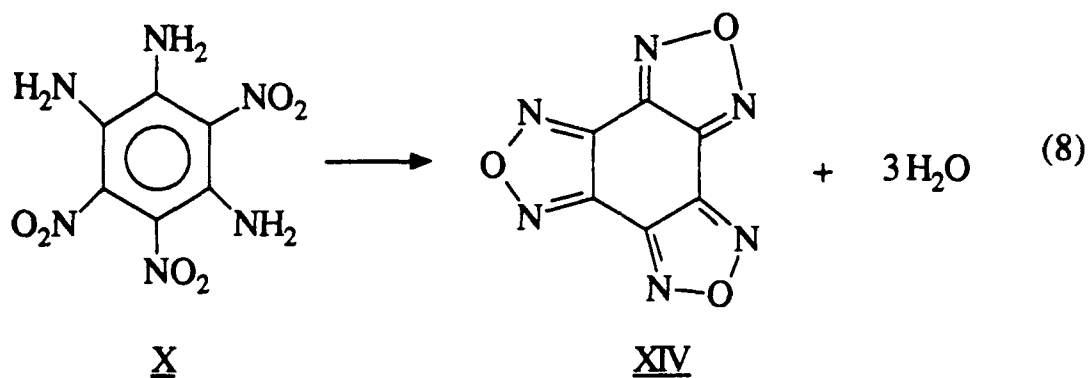
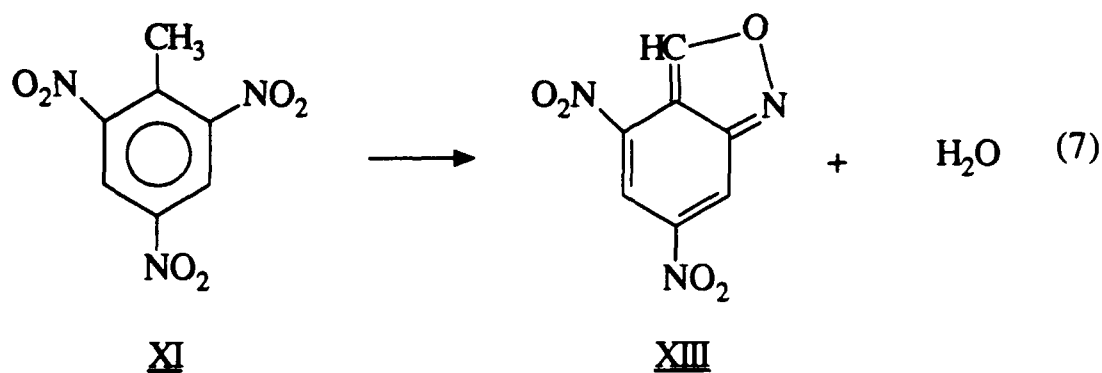
XI, TNT



XII

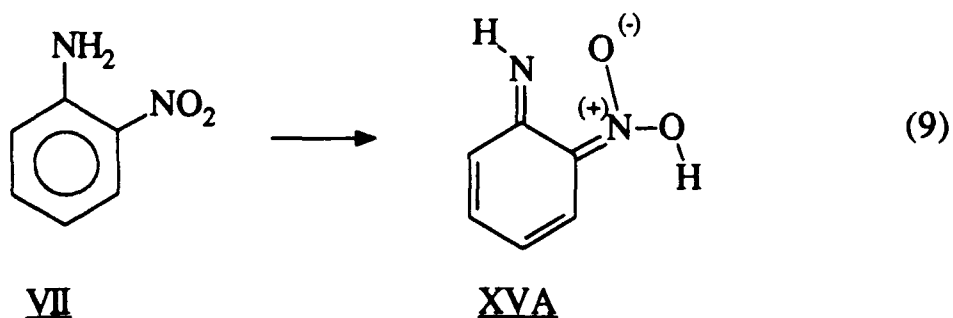
taken as models for the larger trinitroaromatics 1,3,5-triamino-2,4,6-trinitrobenzene (TATB, X), 2,4,6-trinitrotoluene (TNT, XI) and 2,4,6-trinitrocumene (XII). One of our objectives has been to gain insight into factors giving rise to the very different thermal, shock and impact sensitivities of TATB (X) and the alkyltrinitroaromatics XI and XII. TNT (XI), for example, is thermally labile, self-igniting at temperatures between 200 and 210°C (Reference 32), and has intermediate impact and shock sensitivities (References 32 and 39) as does also XII (Reference 40). TATB (X), on the other hand, is stable to temperatures well beyond 300°C (Reference 41) and is so insensitive to impact and shock (References 32 and 39) as to be impractical as an explosive.

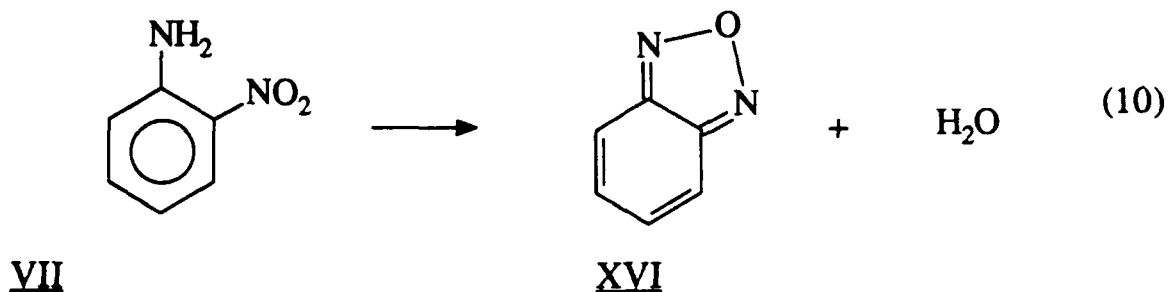
The decompositions of TATB and TNT have been studied extensively, using a variety of experimental techniques (References 15,18,19 and 42-51). Most of the studies of TNT point to reactions involving a methyl hydrogen as being involved in the initial steps of its decomposition (References 42-45, 47 and 49), as contrasted to simple C-NO₂ bond rupture (Reference 19). Evidence for the formation of an intramolecular five-membered ring (dinitroanthranil, XIII), as shown in equation (7), has been reported in low temperature studies of TNT (under 300°C) (References 42 and 43). Five-membered ring formation giving furazans has been reported in



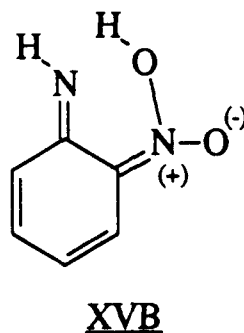
thermal decomposition (Reference 48) and underwater shock and impact (Reference 50) studies of TATB [e.g. as given by equation (8)]. These studies led us to investigate analogous intramolecular ring formation processes for our model systems VII and VIII, as well as possible hydrogen transfer reactions for VII - IX.

We will discuss initially our computed results for the hydrogen transfer and intramolecular ring formation reactions of *o*-nitroaniline, VII. The products, XVA and XVI, are shown below in equations (9) and (10). It is important to point out that no local energy minimum was found





computationally corresponding to the nitronic acid tautomer XVB of *o*-nitroaniline (Reference 34).



Our calculated energies for *o*-nitroaniline and the related systems XVA and XVI are given in Table 3. The tautomerization of VII to produce the nitronic acid XVA is calculated to be endothermic by +39.8 kcal/mole at the 3-21G level. For comparison, the energy change associated with the conversion of *o*-nitrophenol to its nitronic acid tautomer V [equation (5)] was found to +15.4 kcal/mole at the same computational level (Reference 34). Our results suggest, therefore, that the formation of XVA is highly unfavored. However the conversion of VII to benzofurazan (XVI) and water has a calculated ΔE of +5.3 kcal/mole. Thus the formation of XVI is calculated to be a nearly neutral thermochemical reaction. This neutral thermochemistry is in accord with earlier speculation concerning the basis for the high thermal stability and very low shock and impact sensitivities of TATB (Reference 52). It has been suggested that its stability reflects the fact that the steps producing furazan derivatives of TATB (e.g. XIV) are thermodynamically nearly neutral (Reference 52), resulting in little or no early release of energy to drive subsequent decomposition steps.

Our findings for *o*-nitrotoluene (VIII) and related reaction products differ considerably from those for *o*-nitroaniline. First, the hydrogen transfer isomer of VIII is not a nitronic acid, but instead contains an intramolecular ring, XVII. It is noteworthy that these computations were begun at several different starting geometries, each involving a methyl hydrogen transferred to a nitro oxygen atom. When the hydrogen was initially placed on the closer oxygen, the parent

TABLE 3. CALCULATED 3-21G ENERGIES

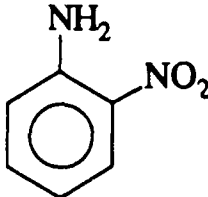
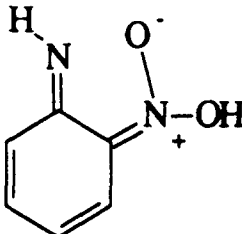
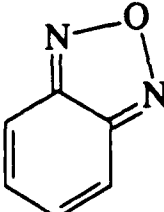
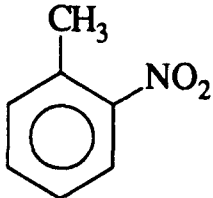
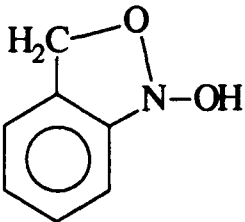
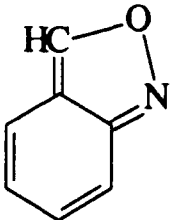
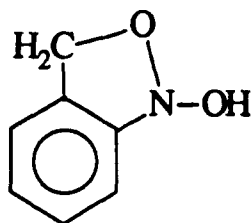
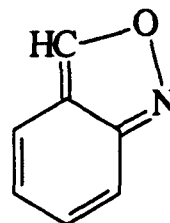
Molecule	Total Energy (hartrees)	Relative Energy (kcal/mole)
1. <u><i>o</i>-Nitroaniline (VII)</u> <u>and related systems:</u>		
<u>VII</u> 	-486.44531	0.0
<u>XVA</u> 	-486.38182	+39.8
<u>XVI</u> 	-410.85083	-----
<u>XVI</u> + H ₂ O	-486.43679	+5.3

TABLE 3. CALCULATED 3-21G ENERGIES (Concluded).

	Molecule	Total Energy (hartrees)	Relative Energy (kcal/mole)
2. <u><i>o</i>-Nitrotoluene (VIII)</u> and related systems:			
<u>VIII</u>		-470.53030	0.0
<u>XVII</u>		-470.56318	-20.6
<u>XVIII</u>		-394.99237	-----
	<u>XVIII</u> + H ₂ O	-470.57833	-30.1



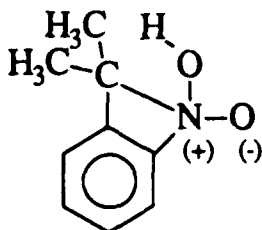
XVII



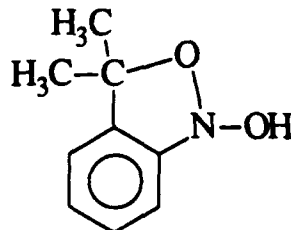
XVIII

molecule, *o*-nitrotoluene, was regenerated computationally. However when the hydrogen was placed on the more distant nitro oxygen, the bicyclic nonplanar **XVII** was formed. As shown in Table 3, the formation of **XVII** from **VIII** is exothermic by -20.6 kcal/mole (at the 3-21G level). The further reaction of **XVII** to form anthranil (**XVIII**) and water is also exothermic by -9.5 kcal/mole. From a thermodynamic standpoint, therefore, the formation of both **XVII** and **XVIII** from **VIII** is predicted to be highly favored. Energy released by forming such products could help to stimulate further decomposition steps. This is consistent with experimental evidence indicating that a decay product of the larger trinitroaromatic **XI** resulting from a methyl hydrogen bond rupture accumulates to a threshold level and then catalytically initiates its continuing exothermic thermochemical decomposition (Reference 44).

In our investigation of *o*-nitrocumene (**IX**) and its possible α -hydrogen transfer products, we have found local energy minima for a thermodynamically unfavored bicyclic system **XIX** and a



XIX

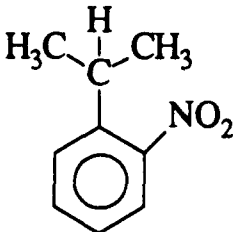
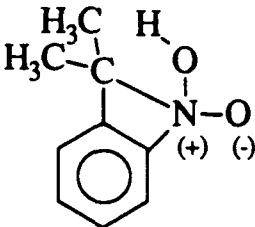
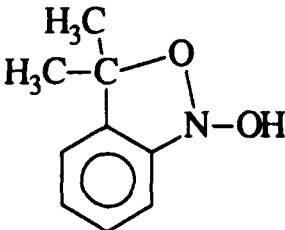


XX

thermodynamically favored bicyclic system **XX**. Our STO-3G energies for **IX**, **XIX** and **XX** are given in Table 4. As in the case of *o*-nitrotoluene, no local energy minima were found for nitronic acid tautomers of **IX**.

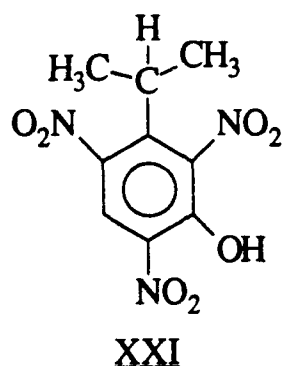
XX is analogous to the hydrogen transfer product **XVII**, formed from *o*-nitrotoluene. In view of this and the fact that 2,4,6-trinitrocumene and TNT have similar structural features and impact sensitivities (Reference 40), it is conceivable that the decomposition of **XII** may follow a path initially analogous to that of TNT, involving the rupture of a C-H(α) bond rather than a C-NO₂ bond.

TABLE 4. CALCULATED STO-3G ENERGIES
OF *O*-NITROCUMENE AND RELATED SYSTEMS ^a

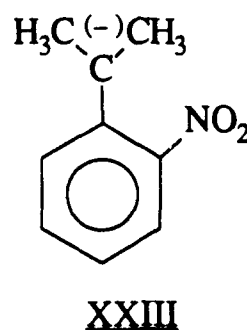
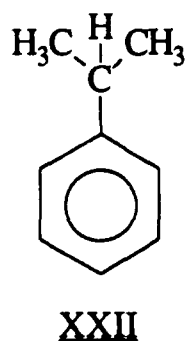
Molecule	Total Energy (hartrees)	Relative Energy (kcal/mole)
<div>IX</div> <div></div>	-544.33928	0.0
<div>XIX</div> <div></div>	-544.30219	+23.3
<div>XX</div> <div></div>	-544.44505	-66.4

^aIt should be noted that the STO-3G procedure tends to somewhat overestimate the magnitudes of reaction energies.

Our studies relating to 2,4,6-trinitrocumene have also focused on an interesting feature of its x-ray crystal data, which show a planar isopropyl group with relatively short C-CH₃ bond distances (1.418 Å, instead of the typical 1.53 Å) (Reference 53). Gilardi et al have suggested that the apparently planar isopropyl group and shortened C-CH₃ bond distances found in the crystal structure of **XII** may be a result of turning or flip-flopping by a pyramidal isopropyl group, producing a superpositioning effect in the crystal structure and giving the appearance of a planar isopropyl group with seemingly shortened C-CH₃ distances (References 53 and 54). The crystal structure for a similar molecule, 3-hydroxy-2,4,6-trinitrocumene (**XXI**), which (unlike **XII**) has no axis of symmetry, shows a pyramidal isopropyl group with normal C-CH₃ bond distances



(Reference 23). In order to clarify the uncertainty concerning the structure of **XII**, we computed optimized gas phase structures of isopropyl benzene (**XXII**), 2,4,6-trinitrocumene (**XII**), *o*-nitrocumene (**IX**) and the carbanion **XXIII** of *o*-nitrocumene. All were found to have pyramidal isopropyl groups



with normal C-CH₃ bond lengths. On the basis of our calculations and the other available evidence, we conclude that the isopropyl group of **XII** in its crystalline form is in fact pyramidal. In this context, it is relevant to point out that both UV (Reference 55) and NMR (Reference 53) studies indicate that the isopropyl group of 2,4,6-trinitrocumene in solution is pyramidal.

SECTION III

CONCLUDING REMARKS

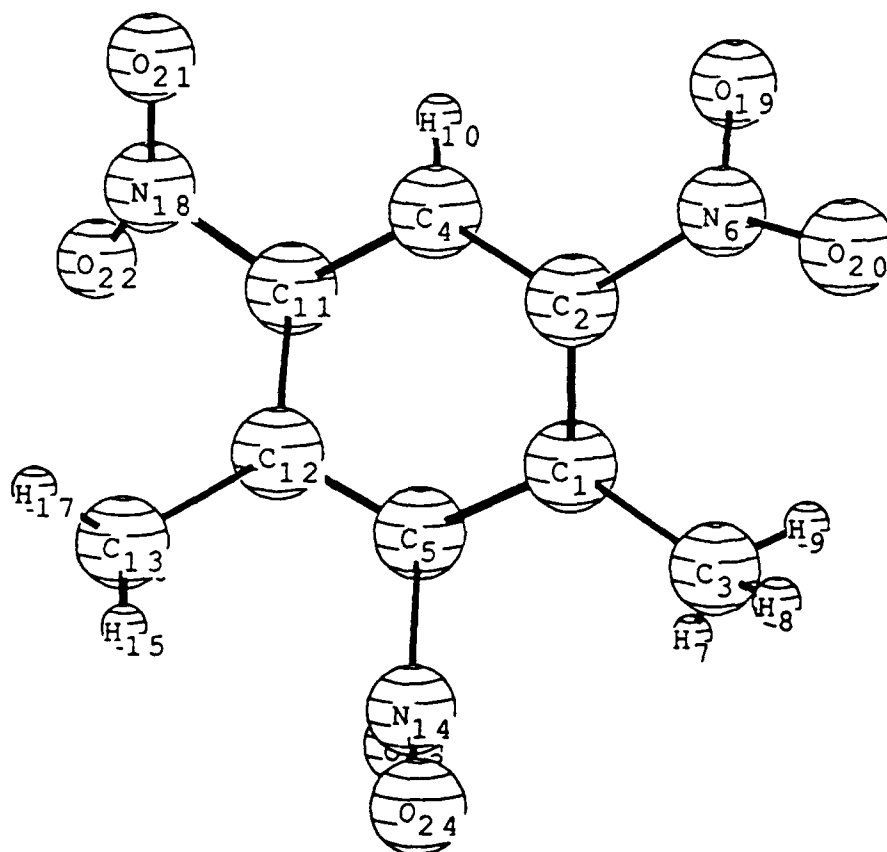
The search for a better understanding of which molecular properties are important in determining the sensitivities of energetic materials to outside stimuli is an important objective of high energy materials research, and reflects a need for the development of less sensitive munitions. In this project, considerable progress has been made in understanding factors which influence sensitivity within separate classes of highly energetic systems. For example, our relationship between $V_{\text{mid, max}}$ and impact sensitivity for a group of eighteen nitroaromatics suggests that the instability associated with the weakest C-NO₂ linkage in nitroaromatics may be a key factor involved in the initiation of decomposition by impact.

Molecules which do not fit the existing correlations suggest starting points for further investigations aimed at elucidating the basis for their exceptional behavior. This was the driving force for our computational studies relating to hydroxynitroaromatics, which led to our suggestion that the high sensitivities of these compounds may be due to the formation of small quantities of unstable nitronic acid tautomers. We have also investigated possible α -hydrogen transfer and intramolecular ring formation reactions of model systems representing the very insensitive TATB and the alkyl-substituted trinitroaromatics TNT and 2,4,6-trinitrocumene, which have intermediate impact sensitivities but are thermally quite unstable. Our results are consistent with earlier speculation and experimental studies of TATB and TNT.

APPENDIX A
2,4,6-TRINITRO-m-XYLENE

The short distances between non-bonded hydrogens and oxygens are H10-O21 (2.50 Å), H10-O19 (2.50 Å), H17-O22 (2.49 Å), and H9-O20 (2.49 Å).

The N6, N14, and N18 nitro groups are rotated out of the mean plane of the benzene ring by approximately 34°, 36° and 75°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.394000 (1)					
3	3	C	1	1.495000 (2)	2	124.600 (24)			
4	4	C	2	1.374000 (3)	1	122.400 (25)	3	174.800 (46)	0
5	5	C	1	1.383000 (4)	2	114.200 (26)	4	-1.700 (47)	0
6	6	N	2	1.474000 (5)	1	120.800 (27)	3	-7.900 (48)	0
7	7	H	3	0.919000 (6)	1	111.800 (28)	2	-137.400 (49)	0
8	8	H	3	1.013000 (7)	1	113.500 (29)	2	85.800 (50)	0
9	9	H	3	0.933000 (8)	1	117.000 (30)	5	151.800 (51)	0
10	10	H	4	0.799000 (9)	2	120.300 (31)	1	-179.100 (52)	0
11	11	C	4	1.374000 (10)	2	119.500 (32)	6	-176.500 (53)	0
12	12	C	5	1.383000 (11)	1	127.200 (33)	3	-175.800 (54)	0
13	13	C	12	1.495000 (12)	5	121.100 (34)	1	-175.800 (55)	0
14	14	N	5	1.480000 (13)	12	116.400 (35)	13	4.200 (56)	0
15	15	H	13	0.919000 (14)	12	111.800 (36)	5	38.800 (57)	0
16	16	H	13	1.013000 (15)	12	113.500 (37)	5	-98.000 (58)	0
17	17	H	13	0.933000 (16)	12	117.000 (38)	11	-24.400 (59)	0
18	18	N	11	1.474000 (17)	4	116.700 (39)	2	-176.500 (60)	0
19	19	O	6	1.220000 (18)	2	116.700 (40)	1	146.400 (61)	0
20	20	O	6	1.223000 (19)	2	118.200 (41)	1	-34.900 (62)	0
21	21	O	18	1.220000 (20)	11	116.700 (42)	4	-36.200 (63)	0
22	22	O	18	1.223000 (21)	11	118.200 (43)	4	142.600 (64)	0
23	23	O	14	1.212000 (22)	5	117.400 (44)	1	-104.400 (65)	0
24	24	O	14	1.212000 (23)	5	117.400 (45)	1	75.600 (66)	0

STOICHIOMETRY C8H7N3O6

E= -915.127510152

EIGENVALUES — -0.31340 -0.31323 0.12593 0.14048 0.18917

Estimated ionization potential: 8.5 ev

TOTAL ATOMIC CHARGES.

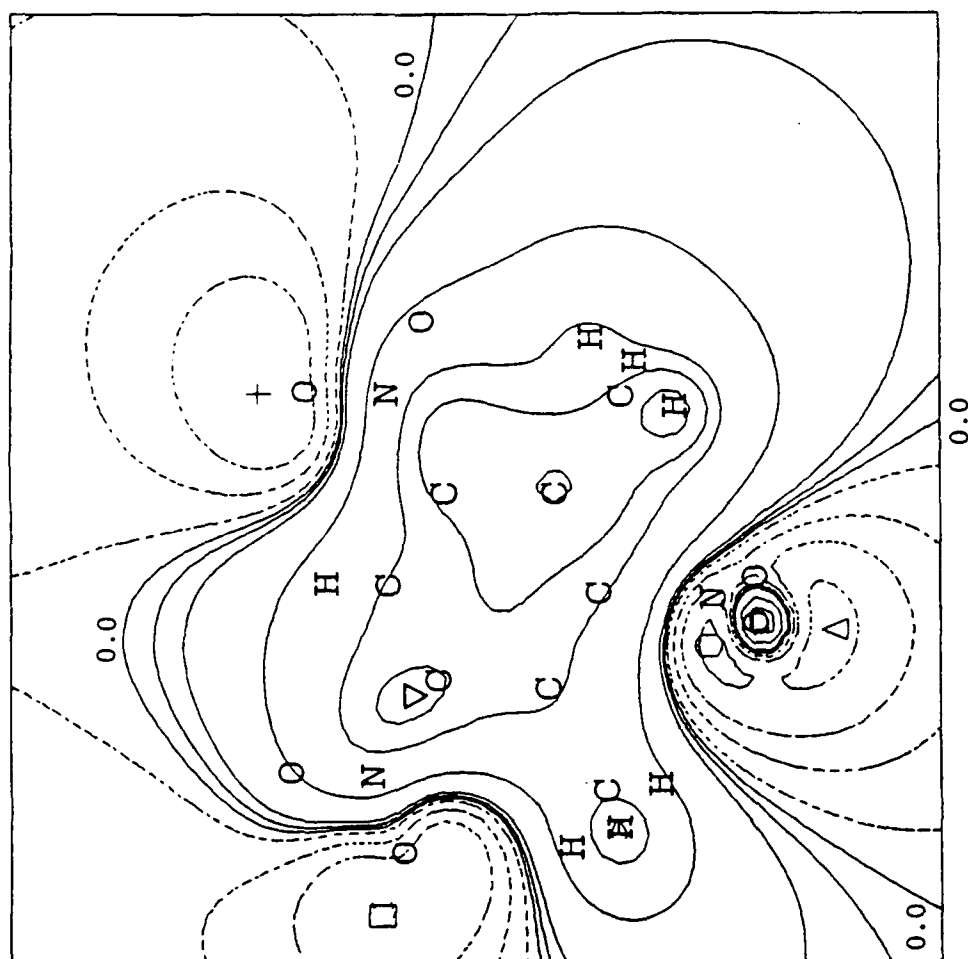
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1	C	5.928368	+0.07
2	C	5.886401	+0.11
3	C	6.341944	-0.34
4	C	6.122008	-0.12
5	C	5.906374	+0.09
6	N	6.829509	+0.17
7	H	0.868199	+0.13
8	H	0.860800	+0.14
9	H	0.858895	+0.14
10	H	0.851523	+0.15
11	C	5.886519	+0.11
12	C	5.928594	+0.07
13	C	6.341918	-0.34
14	N	6.824424	+0.18
15	H	0.868321	+0.13
16	H	0.860840	+0.14
17	H	0.858946	+0.14
18	N	6.829450	+0.17
19	O	8.186679	-0.19
20	O	8.193803	-0.19
21	O	8.186637	-0.19
22	O	8.193737	-0.19
23	O	8.193052	-0.19
24	O	8.193059	-0.19

DIPOLE MOMENT (DEBYE): X=-0.0464 Y=-0.0094 Z=-1.2699 TOTAL= 1.2707

V_{mid}: C₂-N₆: 0.204
 C₁₁-N₁₈: 0.204
 C₅-N₁₄: 0.193

Bond Orders: C₂-N₆: 1.24
 C₁₁-N₁₈: 1.24
 C₅-N₁₄: 1.22
 N₆-O₁₉: 2.09
 N₆-O₂₀: 2.08
 N₁₈-O₂₁: 2.09
 N₁₈-O₂₂: 2.08
 N₁₄-O₂₃: 2.13
 N₁₄-O₂₄: 2.13

-25.1
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-6.3
-1.9
0.0
1.3
3.1
12.6
25.1
28.9
32.6

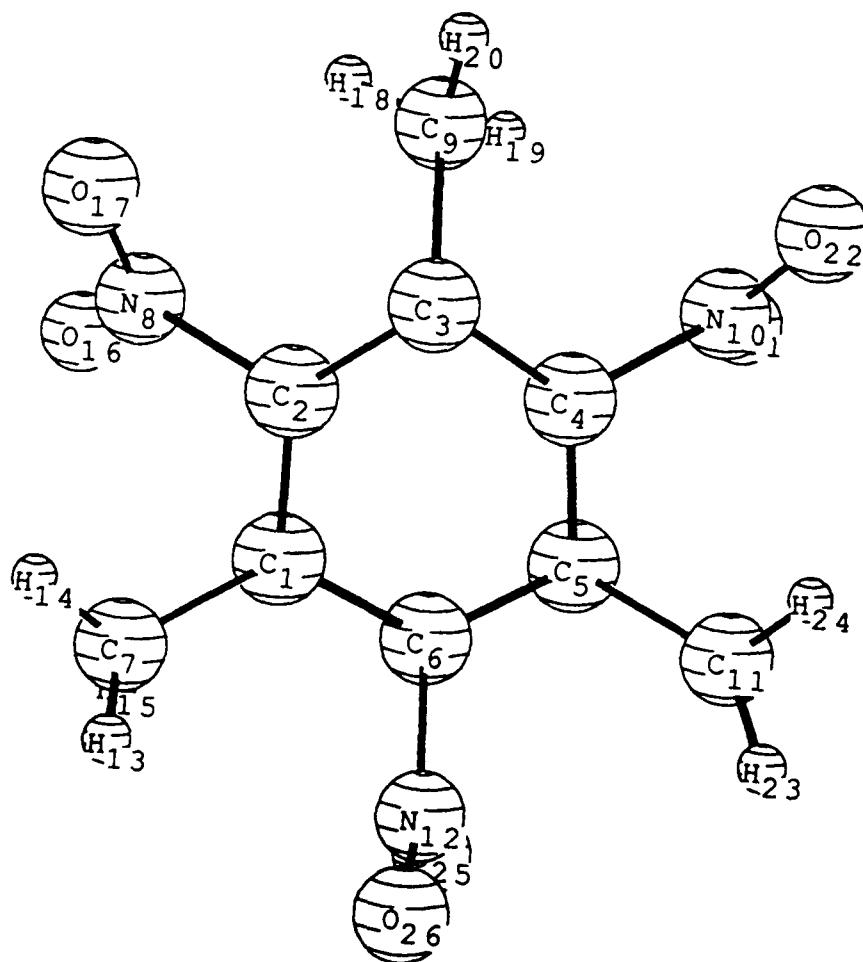


MINIMA	
□	-25.439
○	-30.384
△	-31.168
+	-22.571
MAXIMA	
▽	+29.788

Figure A-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-m-xylene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX B
2,4,6-TRINITROMESITYLENE

The short distances between non-bonded hydrogens and oxygens are H14-O16 (2.54 Å), H13-O27 (2.63 Å) and H18-O17 (2.75 Å). Nitro groups N8, N10 and N12 are rotated out of plane by approximately 68°, 80° and 76° respectively.



				Z-MATRIX (ANGSTROMS AND DEGREES)					
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J

1	1	C							
2	2	C	1	1.395609 (1)					
3	3	C	2	1.386043 (2)	1	125.260 (27)			
4	4	C	3	1.387340 (3)	2	114.727 (28)	1	0.899 (52)	0
5	5	C	4	1.389094 (4)	3	125.634 (29)	2	-0.110 (53)	0
6	6	C	5	1.386824 (5)	4	114.264 (30)	3	-0.629 (54)	0
7	7	C	1	1.505111 (6)	2	122.513 (31)	3	178.507 (55)	0
8	8	N	2	1.476723 (7)	3	117.487 (32)	4	-178.840 (56)	0
9	9	C	3	1.507730 (8)	2	122.827 (33)	1	179.642 (57)	0
10	10	N	4	1.484054 (9)	3	117.243 (34)	2	179.683 (58)	0
11	11	C	5	1.500910 (10)	4	122.514 (35)	3	-178.694 (59)	0
12	12	N	6	1.481970 (11)	1	117.005 (36)	2	179.542 (60)	0
13	13	H	7	0.897467 (12)	1	109.795 (37)	2	-132.567 (61)	0
14	14	H	7	0.920477 (13)	1	113.329 (38)	2	-6.856 (62)	0
15	15	H	7	0.807418 (14)	1	116.825 (39)	2	116.548 (63)	0
16	16	O	8	1.215072 (15)	2	117.178 (40)	1	-67.545 (64)	0
17	17	O	8	1.210455 (16)	2	118.346 (41)	1	112.427 (65)	0
18	18	H	9	0.985381 (17)	3	110.920 (42)	2	-31.431 (66)	0
19	19	H	9	0.976318 (18)	3	110.997 (43)	2	-144.361 (67)	0
20	20	H	9	0.939811 (19)	3	109.776 (44)	2	93.495 (68)	0
21	21	O	10	1.203774 (20)	4	118.137 (45)	5	80.318 (69)	0
22	22	O	10	1.213591 (21)	4	116.823 (46)	5	-99.956 (70)	0
23	23	H	11	0.939811 (22)	5	110.588 (47)	6	-38.348 (71)	0
24	24	H	11	0.900494 (23)	5	113.224 (48)	6	-160.649 (72)	0
25	25	H	11	0.855687 (24)	5	115.770 (49)	6	81.284 (73)	0
26	26	O	12	1.210209 (25)	6	117.689 (50)	1	104.741 (74)	0
27	27	O	12	1.199151 (26)	6	117.799 (51)	1	-75.967 (75)	0

STOICHIOMETRY C9H9N3O6

SCF DONE: E(RHF) = -953.951944215 A.U. AFTER 22 CYCLES

EIGENVALUES -- -0.31278 0.15650 0.16305 0.19396 0.20529

Estimated ionization potential: 8.52 eV

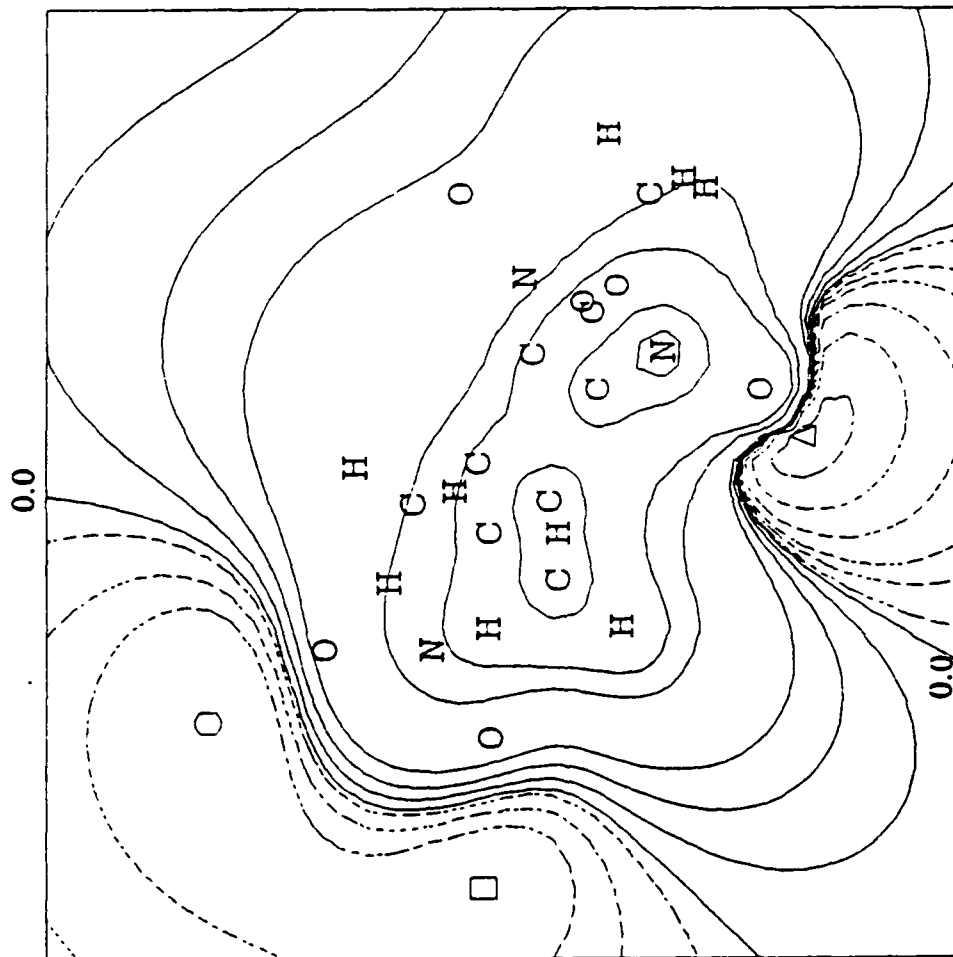
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3 C	5.936049	0.064
4 C	5.912801	0.088
5 C	5.922433	0.078
6 C	5.913981	0.086
7 C	6.448136	-0.448
8 N	6.828167	0.172
9 C	6.309673	-0.690
10 N	6.824056	0.176
11 C	6.407643	-0.408
12 N	6.821455	0.179
13 H	0.835545	0.164
14 H	0.846728	0.153
15 H	0.827870	0.172
16 O	8.196955	-0.197
17 O	8.192877	-0.193
18 H	0.877386	0.123
19 H	0.876473	0.124
20 H	0.864341	0.136
21 O	8.194207	-0.194
22 O	8.197069	-0.197
23 H	0.855237	0.145
24 H	0.851193	0.149
25 H	0.837340	0.163
26 O	8.196696	-0.197
27 O	8.197903	-0.198

DIPOLE MOMENT (DEBYE): X= 0.0817 Y=-0.0475 Z= 0.0520 TOTAL= 0.1078

V-mid: N8-C2: 0.186
 N10-C4: 0.188
 N12-C6: 0.189

Bond Order: N8-C2: 1.22
 N10-C4: 1.20
 N12-C6: 1.21
 O17-N8: 1.96
 O18-N8: 1.98
 O21-N10: 2.02
 O22-N10: 1.97
 O26-N12: 1.99
 O27-N12: 2.04

0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 62.751
 313.754
 627.509
 0.000

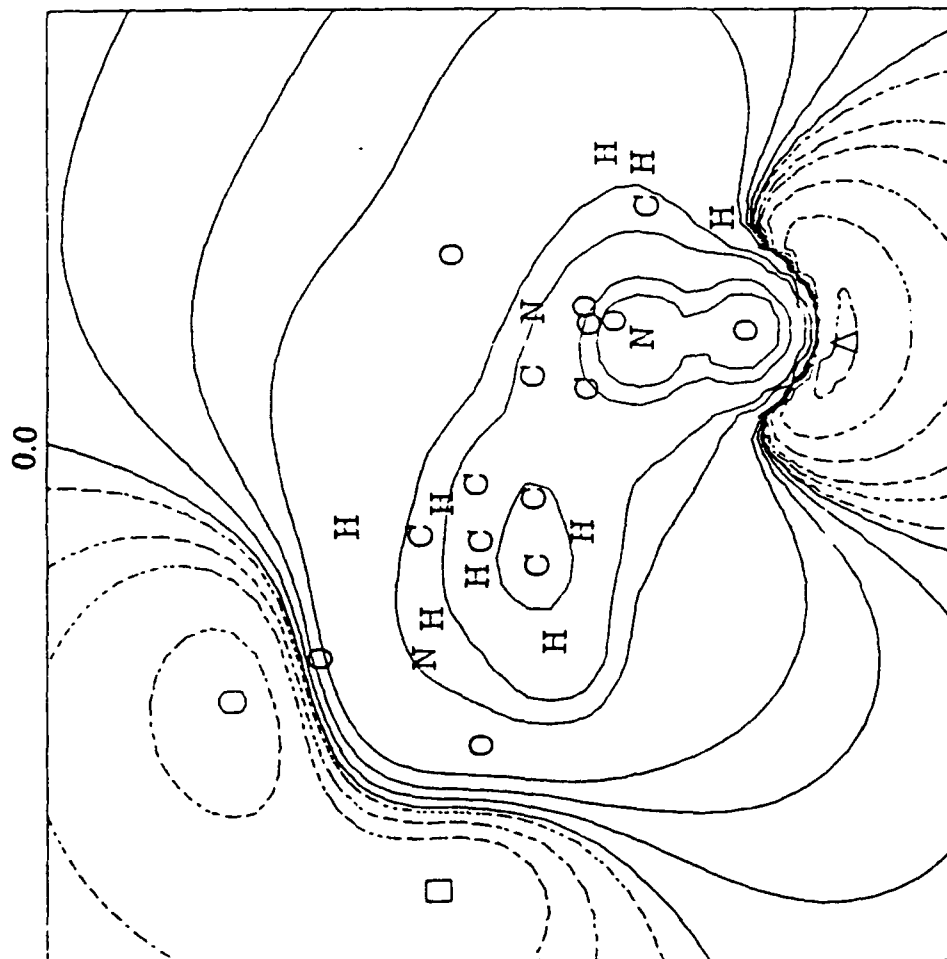


MINIMA

□ -4.700
 ○ -5.547
 △ -33.158

Figure B-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroresorcinol, in the plane 1.75 Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 62.751
 313.754
 627.509
 0.000



MINIMA

□ -4.838
 ○ -8.283
 Δ -28.432

Figure B-2.

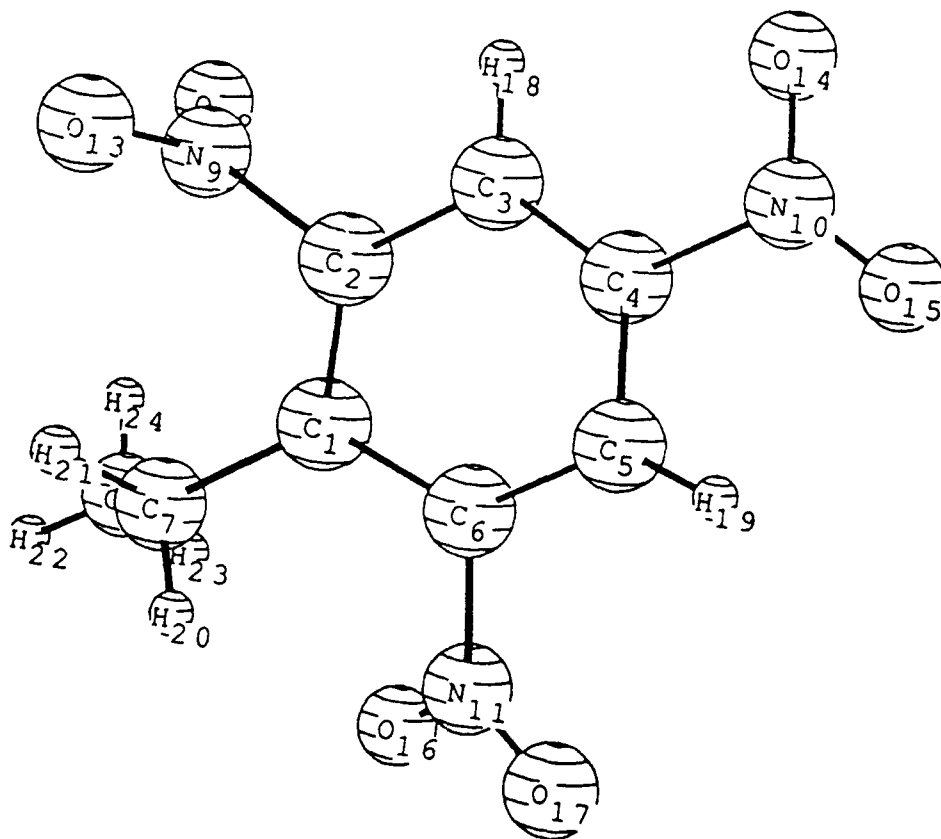
Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenylene, in the plane 1.75Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX C

2,4,6-TRINITROETHYLBENZENE

The short distances between non-bonded hydrogens and oxygens are H18-O14 (2.43 Å), H19-O15 (2.35 Å), H20-O16 (2.43 Å) and H21-O13 (2.50 Å).

The N10 nitro group is rotated by only about 6°, while the other nitro groups are both rotated by more than 50° (N9 ~ 63° and N11 ~ 51°).



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.380000 (1)					
3	3	C	2	1.400036 (2)	1	124.138 (24)			
4	4	C	3	1.346180 (3)	2	117.570 (25)	1	-3.060 (46)	0
5	5	C	4	1.397462 (4)	3	123.238 (26)	2	0.463 (47)	0
6	6	C	5	1.367845 (5)	4	115.552 (27)	3	3.213 (48)	0
7	7	C	1	1.505557 (6)	2	123.639 (28)	3	-177.818 (49)	0
8	8	C	7	1.531437 (7)	1	112.348 (29)	2	76.921 (50)	0
9	9	N	2	1.458938 (8)	3	115.966 (30)	4	177.472 (51)	0
10	10	N	4	1.491610 (9)	5	116.888 (31)	6	-178.171 (52)	0
11	11	N	6	1.479831 (10)	5	113.743 (32)	4	176.560 (53)	0
12	12	O	9	1.215648 (11)	2	118.028 (33)	3	62.726 (54)	0
13	13	O	9	1.214990 (12)	2	118.662 (34)	3	-115.532 (55)	0
14	14	O	10	1.233005 (13)	4	114.830 (35)	5	172.910 (56)	0
15	15	O	10	1.196704 (14)	4	119.125 (36)	5	-5.044 (57)	0
16	16	O	11	1.214990 (15)	6	118.365 (37)	5	-129.708 (58)	0
17	17	O	11	1.215648 (16)	6	117.347 (38)	5	50.922 (59)	0
18	18	H	3	0.999000 (17)	2	118.732 (39)	1	177.032 (60)	0
19	19	H	5	0.943875 (18)	4	115.541 (40)	3	-165.104 (61)	0
20	20	H	7	0.958645 (19)	1	108.895 (41)	2	-162.317 (62)	0
21	21	H	7	0.958645 (20)	1	109.240 (42)	2	-43.190 (63)	0
22	22	H	8	0.956504 (21)	7	115.751 (43)	1	-177.865 (64)	0
23	23	H	8	0.961509 (22)	7	103.014 (44)	1	63.451 (65)	0
24	24	H	8	0.951525 (23)	7	108.837 (45)	1	-52.805 (66)	0

STOICHIOMETRY C8H7N3O6

SCF DONE: E(RHF) = -915.264040980

EIGENVALUES — -0.31648 -0.31536 0.12440 0.13591 0.18671

Estimated ionization potential: 8.59 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.940839	0.059
2	C	5.897024	0.103
3	C	6.054537	-0.055
4	C	5.893531	0.106
5	C	6.071561	-0.072
6	C	5.895058	0.105
7	C	6.174044	-0.174
8	C	6.295210	-0.295
9	N	6.831461	0.169
10	N	6.819867	0.180
11	N	6.827034	0.173
12	O	8.189975	-0.190
13	O	8.192135	-0.192
14	O	8.198018	-0.198
15	O	8.186915	-0.187
16	O	8.195772	-0.196
17	O	8.190246	-0.190
18	H	0.860837	0.139
19	H	0.852713	0.147
20	H	0.886131	0.114
21	H	0.881087	0.119
22	H	0.885397	0.115
23	H	0.885462	0.115
24	H	0.895142	0.105

DIPOLE MOMENT (DEBYE): X=-0.9287 Y= 0.0689 Z=-0.6332 TOTAL= 1.1262

Bond Order: C2-N9: 1.27

V-mid: C2-N9: 0.197

C4-N10: 1.18

C4-N10: 0.203

C6-N11: 1.21

C6-N11: 0.199

N9-O12: 1.96

N9-O13: 1.96

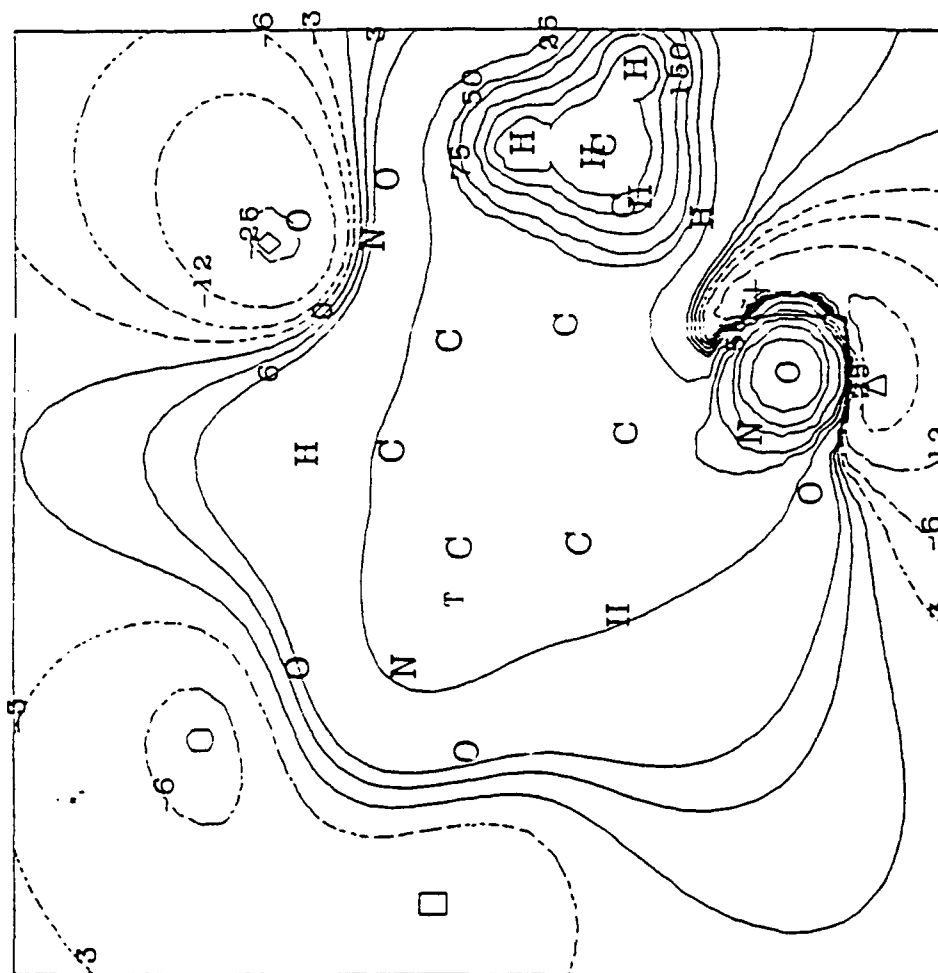
N10-O14: 1.88

N10-O15: 2.05

N11-O16: 1.96

N11-O17: 1.96

-25.0
 -12.0
 -6.0
 -3.0
 0.0
 3.0
 6.0
 25.0
 50.0
 75.0
 150.0
 300.0
 600.0



MINIMA

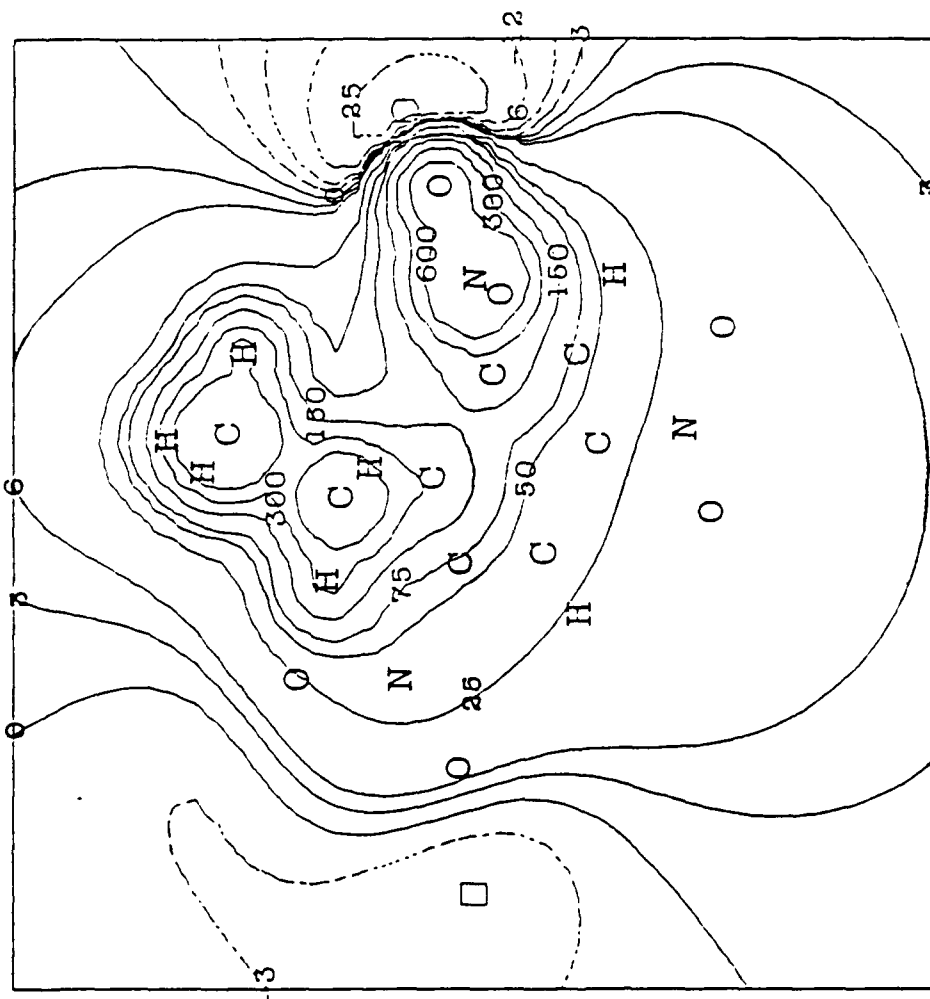
□ -5.503
 ○ -6.896
 △ -41.987
 + -19.804
 ◇ -27.146

MAXIMA

T +34.514

Figure C-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0
300.0
600.0



MINIMA

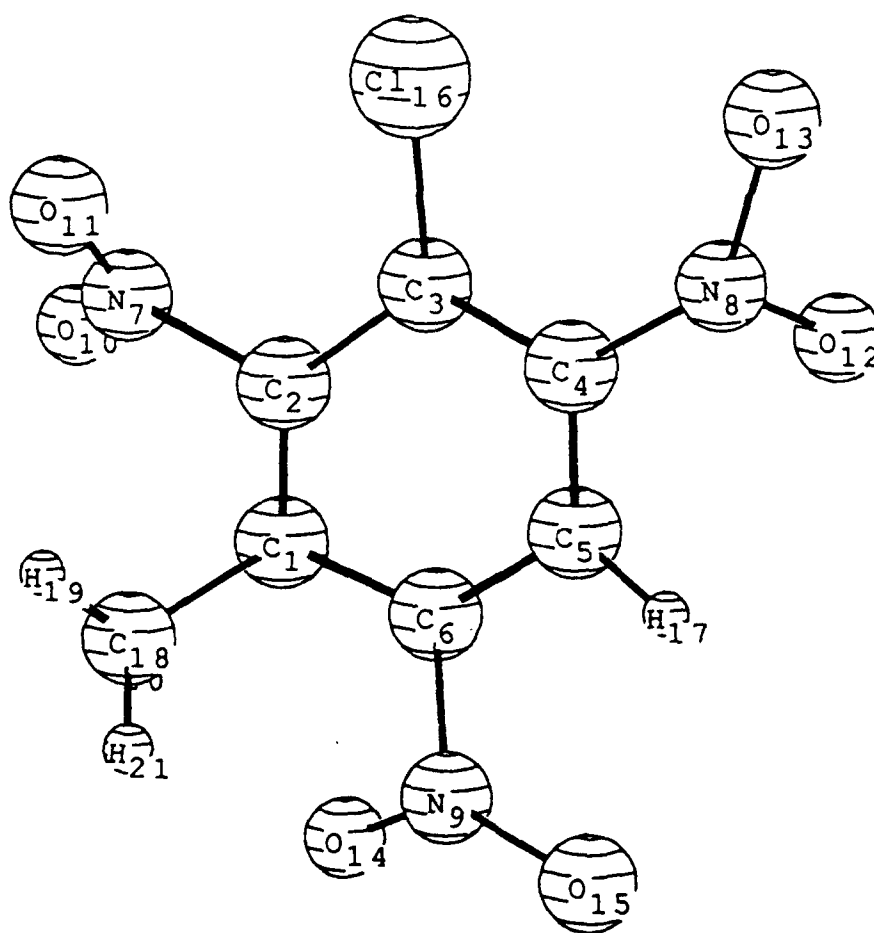
□ -5.353
○ -37.933

Figure C-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX D
3-CHLORO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H21-O14 (2.41 Å) and H17-O15 (2.23 Å).

The N8 and N9 nitro groups are both rotated by approximately 35°, while the N7 nitro group is rotated by more than 80°.



Z-MATRIX (ANGSTROMS AND DEGREES)							
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3 Beta/Z J
1	1	C					
2	2	C	1	1.338000(1)			
3	3	C	2	1.431227(2)	1	125.709(21)	
4	4	C	3	1.392368(3)	2	115.670(22)	1 -4.255(40) 0
5	5	C	4	1.397305(4)	3	120.647(23)	2 5.006(41) 0
6	6	C	5	1.352392(5)	4	119.011(24)	3 -4.079(42) 0
7	7	N	2	1.493255(6)	3	115.308(25)	4 -178.749(43) 0
8	8	N	4	1.422590(7)	5	115.670(26)	6 175.975(44) 0
9	9	N	6	1.523058(8)	5	117.187(27)	4 -178.672(45) 0
10	10	O	7	1.269114(9)	2	118.481(28)	3 104.866(46) 0
11	11	O	7	1.177459(10)	2	114.795(29)	3 -80.214(47) 0
12	12	O	9	1.177940(11)	4	121.200(30)	3 -144.258(48) 0
13	13	O	1	1.243590(12)	4	118.718(31)	3 35.657(49) 0
14	14	O	9	1.199396(13)	6	117.118(32)	5 -141.221(50) 0
15	15	O	9	1.255951(14)	6	113.854(33)	5 34.945(51) 0
16	16	Cl	3	1.71444(15)	4	123.246(34)	5 179.843(52) 0
17	17	H	5	1.012224(16)	4	133.416(35)	3 -174.849(53) 0
18	18	C	1	1.495997(17)	2	123.104(36)	3 179.209(54) 0
19	19	H	18	0.960230(18)	1	109.426(37)	2 -20.452(55) 0
20	20	H	18	0.959922(19)	1	109.476(38)	2 99.587(56) 0
21	21	H	18	0.958896(20)	1	109.444(39)	2 -140.413(57) 0

STOICHIOMETRY C7H4ClN3O6

SCF DONE: E(RHF) = -1333.56294463 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.30955 0.10873 0.13643 0.17527 0.19758

Estimated ionization potential: 8.43 eV

Total atomic charges:

1
 1 C 0.066131
 2 C 0.095898
 3 C 0.061032
 4 C 0.105502
 5 C -0.051140
 6 C 0.097191
 7 N 0.171478
 8 N 0.169550
 9 N 0.170954
 10 O -0.199021
 11 O -0.160216
 12 O -0.180358
 13 O -0.195691
 14 O -0.169041
 15 O -0.196948
 16 Cl -0.018883
 17 H 0.149057
 18 C -0.310376
 19 F 0.124371
 20 H 0.141483
 21 H 0.128727

Dipole moment (Debye):

X= 2.2897 Y= 0.7259 Z= -0.1213 Tot= 2.4050

V-mid: C2-N7: 0.189

C4-N8: 0.205

C6-N9: 0.186

Bond Order: C2-N7: 1.18

C4-N8: 1.36

C6-N9: 1.11

N7-O10: 1.72

N7-O11: 2.16

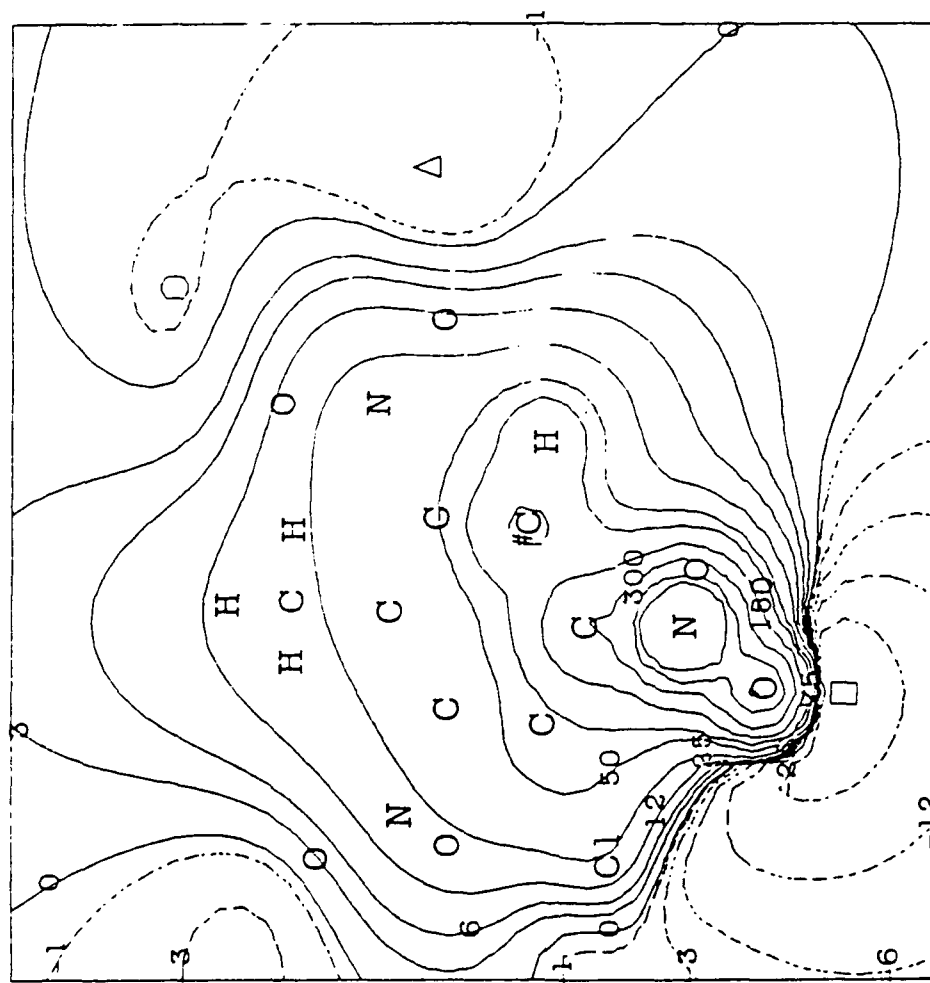
N8-O12: 2.15

N8-O13: 1.83

N9-O14: 2.04

N9-O15: 1.76

-25.0
-12.0
-6.0
-3.0
-1.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA

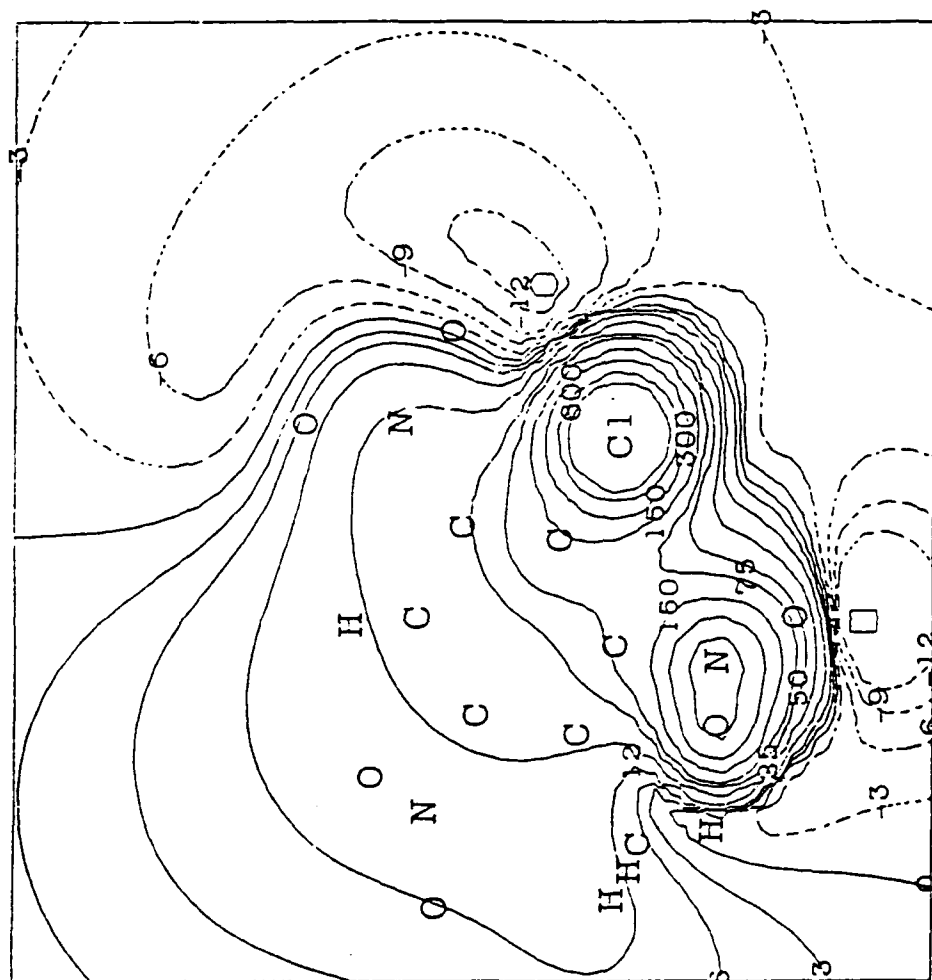
□ -48.9
○ -1.2
△ -2.7

MAXIMA

+167.8

Figure D-1. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-12.0
-9.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA
□ -21.9
○ -13.0

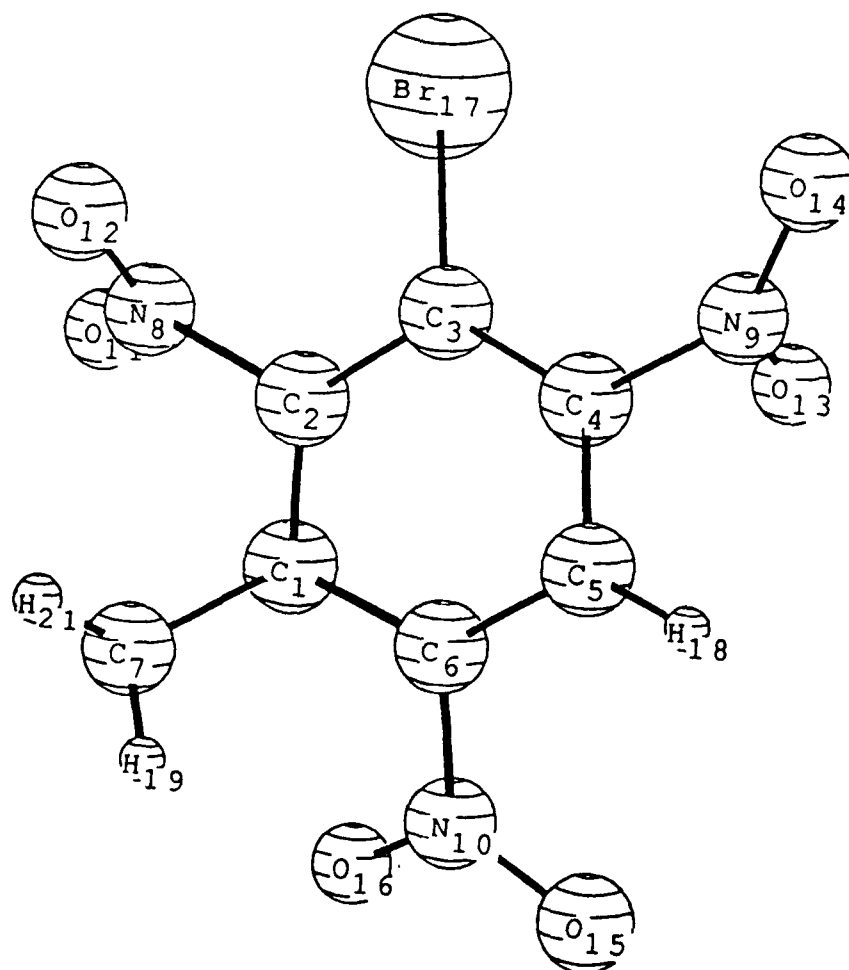
Figure D-2 Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX E

3-BROMO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H18-O15 (2.47 Å) and H19-O16 (2.34 Å).

The N8 nitro group is rotated out of the mean plane of the benzene ring by almost 80°, while the N9 and N1 nitro groups are rotated by about 50° and 37°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
J								
1	1	C						
2	2	C	1	1.391000(1)				
3	3	C	2	1.386831(2)	1	124.752(21)		
4	4	C	3	1.367699(3)	2	117.830(22)	1	-2.954(40)
5	5	C	4	1.405916(4)	3	122.057(23)	2	2.925(41)
6	6	C	5	1.379891(5)	4	117.088(24)	3	-1.195(42)
7	7	C	1	1.501066(6)	2	120.867(25)	3	178.765(43)
8	8	N	2	1.455638(7)	3	118.921(26)	4	179.894(44)
9	9	N	4	1.474076(8)	5	115.988(27)	6	176.831(45)
10	10	N	6	1.465537(9)	5	114.783(28)	4	178.164(46)
11	11	O	8	1.237110(10)	2	116.781(29)	3	100.573(47)
12	12	O	8	1.212164(11)	2	119.976(30)	3	-77.726(48)
13	13	O	9	1.227232(12)	4	116.041(31)	3	-131.017(49)
14	14	O	9	1.192896(13)	4	118.673(32)	3	50.430(50)
15	15	O	10	1.228251(14)	6	118.145(33)	1	-145.222(51)
16	16	O	10	1.213507(15)	6	118.555(34)	1	39.369(52)
17	17	Br	3	1.866842(16)	4	123.075(35)	5	-177.475(53)
18	18	H	5	0.962237(17)	4	121.577(36)	3	178.812(54)
19	19	H	7	0.960260(18)	1	109.064(37)	6	13.932(55)
20	20	H	7	0.966540(19)	1	108.844(38)	6	-105.062(56)
21	21	H	7	0.952576(20)	1	109.759(39)	6	134.493(57)

STOICHIOMETRY C7H4BrN3O6

SCF DONE: E(RHF) = -3434.62662133

Alpha eigenvalues — -0.34376 -0.31921 -0.31638 -0.31605 0.12262

Estimated ionization potential: 8.61 ev

Total atomic charges:

1

1	C	0.081237
2	C	0.092632
3	C	-0.033527
4	C	0.100238
5	C	-0.050166
6	C	0.096820
7	C	-0.317159
8	N	0.159052
9	N	0.179317
10	N	0.166279
11	O	-0.189477
12	O	-0.176590
13	O	-0.195644
14	O	-0.178994
15	O	-0.194100
16	O	-0.189239
17	Br	0.105347
18	H	0.142476
19	H	0.133943
20	H	0.139252
21	H	0.128303

Dipole moment (Debye):

X=	0.7450	Y=	-0.9522	Z=	0.3259	Tot=	1.2522
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Bond Order: C2-N8: 1.28

C4-N9: 1.23

C6-N10: 1.25

N8-O11: 1.86

N8-O12: 1.98

N9-O13: 1.91

N9-O14: 2.07

N10-O15: 1.90

N10-O16: 1.97

V-mid: C2-N8: 0.183

C4-N9: 0.200

C6-N10: 0.190

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0

MINIMA

□ -35.2
○ -7.1
△ -7.1

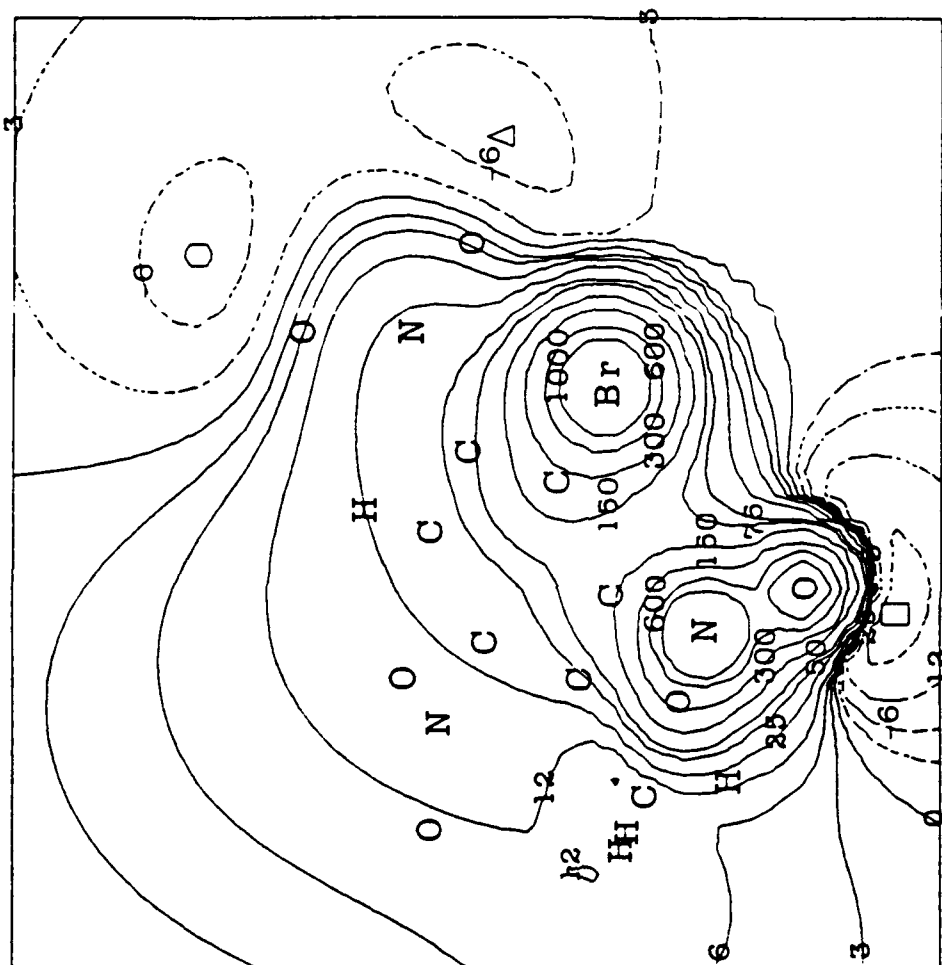


Figure E-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0

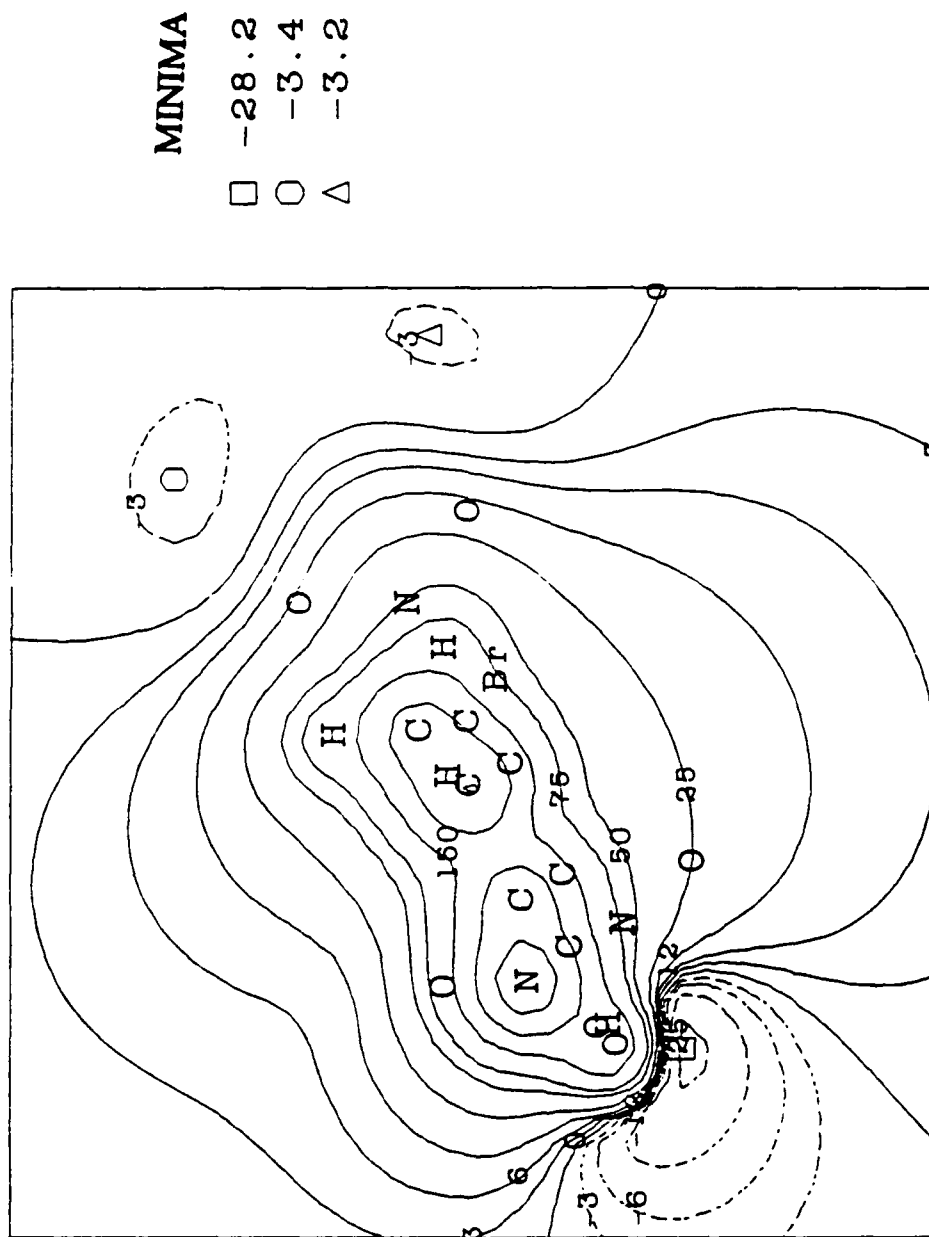
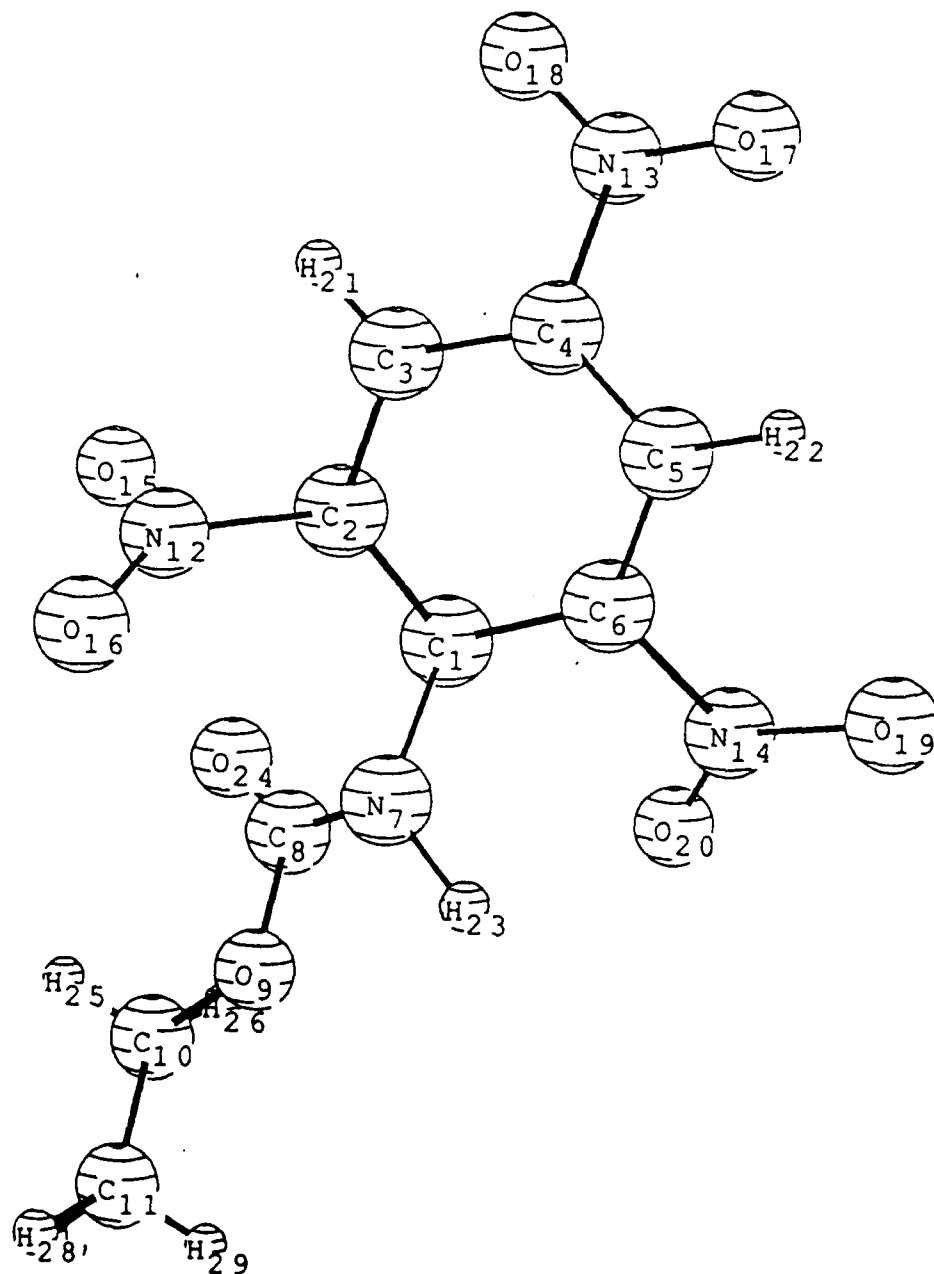


Figure E-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX F
ETHYL(2,4,6-TRINITROPHENYL)CARBAMATE

The short distances between non-bonded hydrogens and oxygens are H21-O18 (2.41 Å), H22-O17 (2.47 Å), H22-O19 (2.49 Å) and H23-O20 (2.47 Å).

The N13 nitro group is rotated out of the mean plane of the benzene ring by approximately 17°, while the N12 and N14 nitro groups are rotated by about 47° and 38°, respectively.



Total atomic charges:

1
 1 C 0.163779
 2 C 0.102747
 3 C -0.049115
 4 C 0.097327
 5 C -0.045397
 6 C 0.084142
 7 N -0.347840
 8 C 0.453964
 9 O -0.266240
 10 C -0.017669
 11 C -0.265862
 12 N 0.183854
 13 N 0.177201
 14 N 0.162719
 15 O -0.190126
 16 O -0.188573
 17 O -0.195429
 18 O -0.187207
 19 O -0.180792
 20 O -0.193106
 21 H 0.144867
 22 H 0.144513
 23 H 0.234194
 24 O -0.323841
 25 H 0.105095
 26 H 0.097999
 27 H 0.098282
 28 H 0.100922
 29 H 0.099590

Dipole moment (Debye):

X= -1.4823 Y= -1.0772 Z= -2.2757 Tot= 2.9217

V-mid:

C2-N12: 0.206
 C4-N13: 0.196
 C6-N14: 0.178

Bond Order:

C2-N12: 1.22
 C4-N13: 1.20
 C6-N14: 1.23
 N12-O15: 1.86
 N12-O16: 2.08
 N13-O17: 1.91
 N13-O18: 1.99
 N14-O19: 1.94
 N14-O20: 1.86

Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.399800(1)					
3	3	C	2	1.393593(2)	1	122.211(29)			
4	4	C	3	1.356650(3)	2	117.976(30)	1	-2.034(56)	0
5	5	C	4	1.392623(4)	3	122.722(31)	2	-0.698(57)	0
6	6	C	5	1.371787(5)	4	117.297(32)	3	4.441(58)	0
7	7	N	1	1.417745(6)	6	122.775(33)	5	-175.318(59)	0
8	8	C	7	1.335253(7)	1	123.100(34)	6	-132.616(60)	0
9	9	O	8	1.326876(8)	7	110.646(35)	1	-177.780(61)	0
10	10	C	9	1.455369(9)	8	115.561(36)	7	-175.735(62)	0
11	11	C	10	1.510133(10)	9	106.304(37)	8	-172.991(63)	0
12	12	N	2	1.477193(11)	3	116.070(38)	4	173.007(64)	0
13	13	N	4	1.485025(12)	5	118.794(39)	6	-175.858(65)	0
14	14	N	6	1.473533(13)	5	115.792(40)	4	172.441(66)	0
15	15	O	12	1.237979(14)	2	116.782(41)	3	45.589(67)	0
16	16	O	12	1.191493(15)	2	118.935(42)	3	-131.685(68)	0
17	17	O	13	1.227110(16)	4	117.538(43)	5	-15.868(69)	0
18	18	O	13	1.210411(17)	4	115.965(44)	5	162.675(70)	0
19	19	O	14	1.218843(18)	6	117.626(45)	5	36.970(71)	0
20	20	O	14	1.237588(19)	6	117.526(46)	5	-140.997(72)	0
21	21	H	3	0.990490(20)	4	121.382(47)	5	-179.820(73)	0
22	22	H	5	0.991278(21)	4	121.110(48)	3	-175.253(74)	0
23	23	H	7	1.103857(22)	1	112.322(49)	2	-144.341(75)	0
24	24	O	8	1.240796(23)	7	124.869(50)	1	2.065(76)	0
25	25	H	10	0.988518(24)	9	110.438(51)	8	-53.410(77)	0
26	26	H	10	0.991278(25)	9	110.198(52)	8	67.654(78)	0
27	27	H	11	0.993518(26)	10	109.272(53)	9	179.887(79)	0
28	28	H	11	0.991666(27)	10	109.485(54)	9	60.027(80)	0
29	29	H	11	0.990416(28)	10	109.612(55)	9	-60.207(81)	0

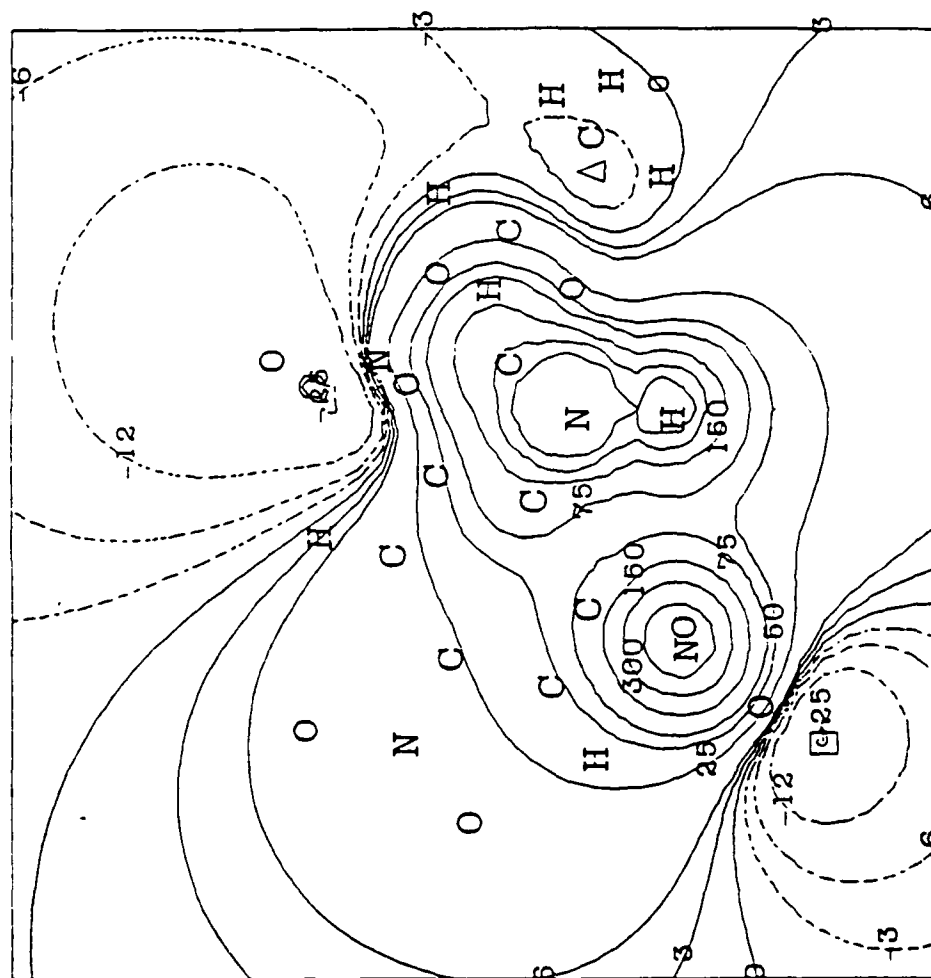
STOICHIOMETRY C9H8N4O8

SCF DONE: E(RHF) = -1156.89781294

EIGENVALUES — -0.31594 -0.30710 0.12151 0.12545 0.18009

Estimated ionization potential: 8.37 ev

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0
300.0
600.0

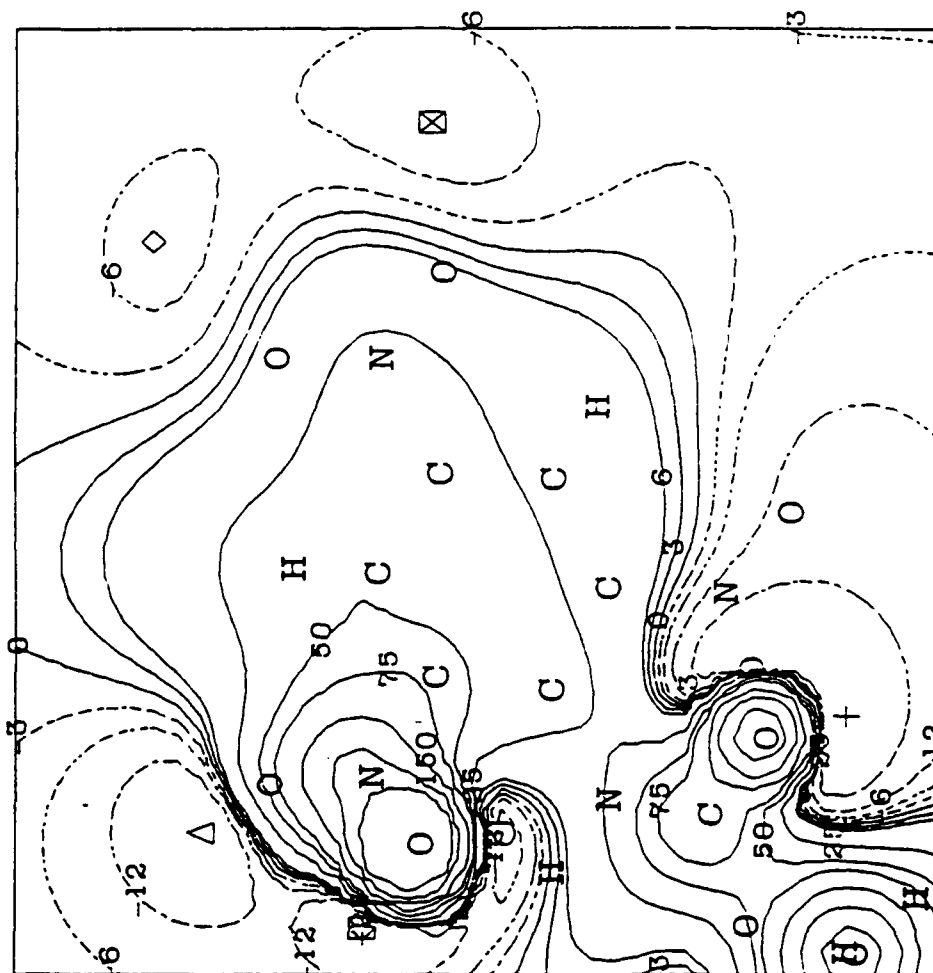


MINIMA

□ -25.464
○ -25.740
△ -4.499

Figure F-1. Calculated electrostatic potential, in kcal/mole, of ethyl(2,4,6-trinitrophenyl)carbamate, in the plane 1.75Å above the N12 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0
300.0
600.0



MINIMA

□ -27.378
○ -19.616
△ -24.253
+ -54.091
◇ -6.871
⊗ -7.674

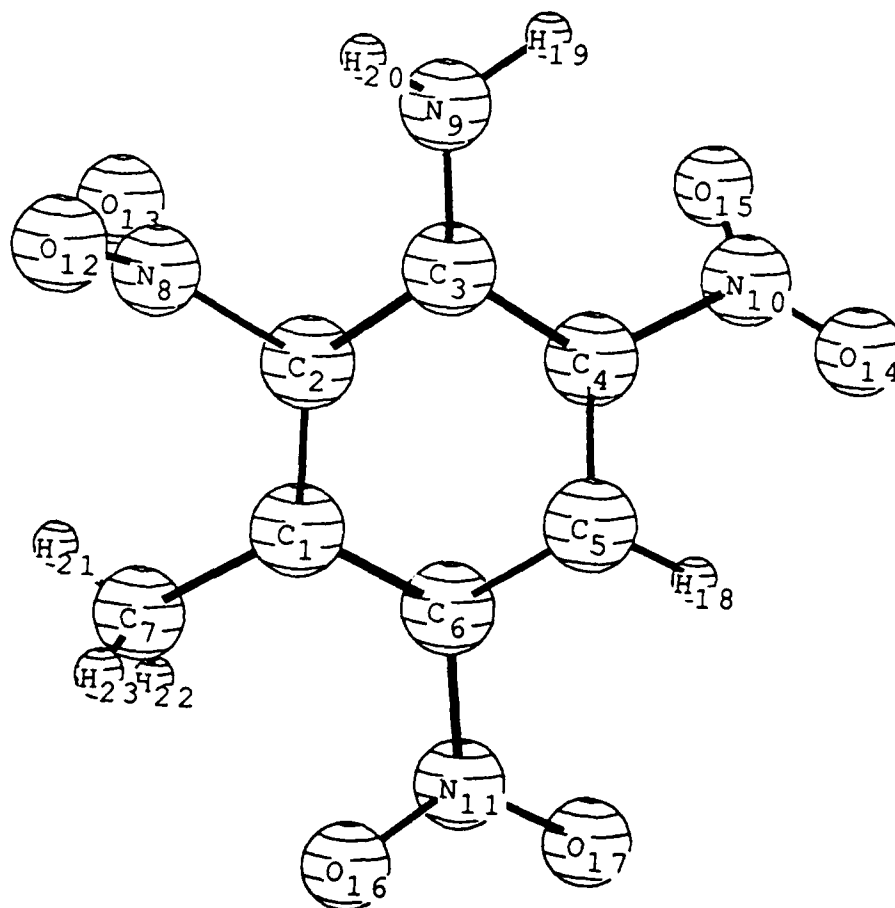
Figure F-2. Calculated electrostatic potential, in kcal/mole, of ethyl(2,4,6-trinitrophenyl)carbamate, in the plane 1.75 Å above the N13 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX G

3-AMINO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H18-O14 (2.38 Å), H19-O15 (2.04 Å), H18-O17 (2.40 Å) and H22-O16 (2.45 Å).

The N8 nitro group is rotated out of the mean plane of the benzene ring by 72°, and the N10 and N11 nitro groups are rotated by 28° and 20°, respectively. The amine group (N9) is rotated by only a few degrees.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTN	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.395000 (1)					
3	3	C	2	1.410838 (2)	1	126.701 (23)			
4	4	C	3	1.402150 (3)	2	114.129 (24)	1	0.979 (44)	0
5	5	C	4	1.378505 (4)	3	122.224 (25)	2	-1.093 (45)	0
6	6	C	5	1.368058 (5)	4	120.320 (26)	3	1.406 (46)	0
7	7	C	1	1.486318 (6)	2	120.905 (27)	3	-179.014 (47)	0
8	8	N	2	1.478266 (7)	3	115.412 (28)	4	-179.582 (48)	0
9	9	N	3	1.356293 (8)	4	124.097 (29)	5	177.944 (49)	0
10	10	N	4	1.452784 (9)	5	116.851 (30)	6	-179.171 (50)	0
11	11	N	6	1.462607 (10)	5	116.091 (31)	4	179.333 (51)	0
12	12	O	8	1.219979 (11)	2	117.040 (32)	1	72.354 (52)	0
13	13	O	8	1.211423 (12)	2	117.381 (33)	1	-108.844 (53)	0
14	14	O	10	1.226476 (13)	4	118.336 (34)	5	-27.908 (54)	0
15	15	O	10	1.225006 (14)	4	119.166 (35)	5	151.840 (55)	0
16	16	O	11	1.218859 (15)	6	119.900 (36)	5	159.673 (56)	0
17	17	O	11	1.227529 (16)	6	117.202 (37)	5	-20.424 (57)	0
18	13	H	5	0.980143 (17)	4	116.582 (38)	3	-179.380 (58)	0
19	19	H	9	0.978715 (18)	3	118.485 (39)	4	3.497 (59)	0
20	20	H	9	0.802824 (19)	3	121.840 (40)	4	-170.689 (60)	0
21	21	H	7	0.950830 (20)	1	112.366 (41)	2	16.885 (61)	0
22	22	H	7	0.915332 (21)	1	110.477 (42)	2	132.601 (62)	0
23	23	H	7	0.949603 (22)	1	110.427 (43)	2	-107.239 (63)	0

STOICHIOMETRY C7H6N4O6

SCF DONE: E(RHF) = -931.120205284 A.U. AFTER 28 CYCLES

EIGENVALUES -- -0.31333 -0.30205 0.13151 0.14777 0.18649

ESTIMATED IONIZATION POTENTIAL: 8.23 ev

TOTAL ATOMIC CHARGES.			
		1	Net Charge
1	C	5.906196	0.014
2	C	5.939706	0.060
3	C	5.797575	0.202
4	C	5.938181	0.062
5	C	6.042300	-0.042
6	C	5.932520	0.067
7	C	6.345575	-0.346
8	N	6.835111	0.165
9	N	7.534281	-0.534
10	N	6.834702	0.165
11	N	6.833735	0.166
12	O	8.195482	-0.195
13	O	8.194229	-0.194
14	O	8.186153	-0.186
15	O	8.214415	-0.214
16	O	8.200247	-0.200
17	O	8.201892	-0.202
18	H	0.854103	0.146
19	H	0.724753	0.275
20	H	0.708393	0.292
21	H	0.870675	0.129
22	H	0.855647	0.144
23	H	0.854132	0.146

DIPOLE MOMENT (DEBYE): X=-1.1727 Y=-0.2785 Z= 1.7132 TOTAL= 2.0947

Vmid: N8-C2: 0.161
 N10-C4: 0.165
 N11-C6: 0.169

BOND ORDER: N8-C2: 1.22
 N10-C4: 1.28
 N11-C6: 1.26
 O12-N8: 1.94
 O13-N8: 1.98
 O14-N10: 1.91
 O15-N10: 1.91
 O16-N11: 1.94
 O17-N11: 1.92

-25.100
 -12.550
 -6.275
 -3.138
 0.000
 3.138
 6.275
 25.100
 50.201
 62.751
 313.754
 627.509
 0.000

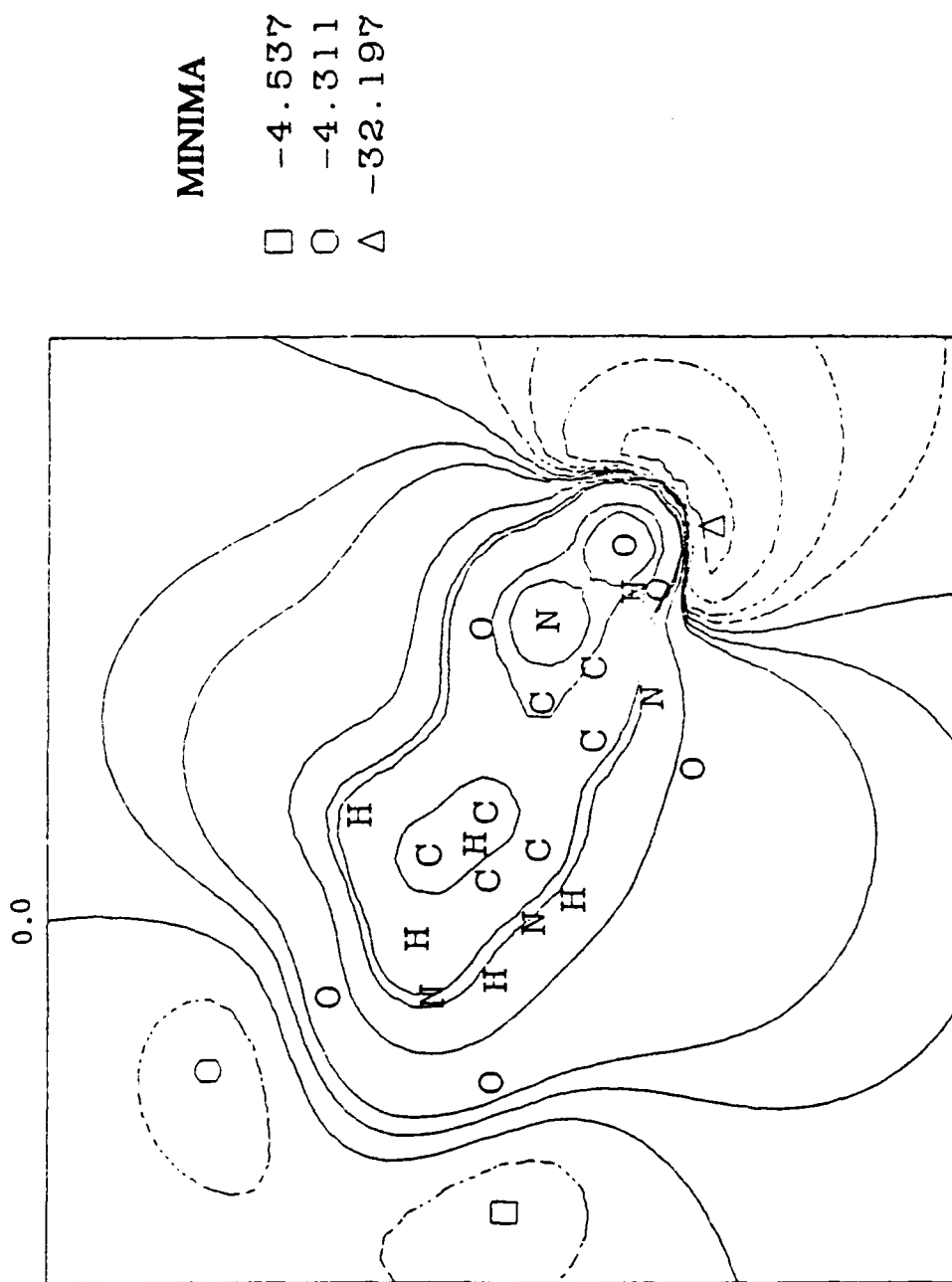
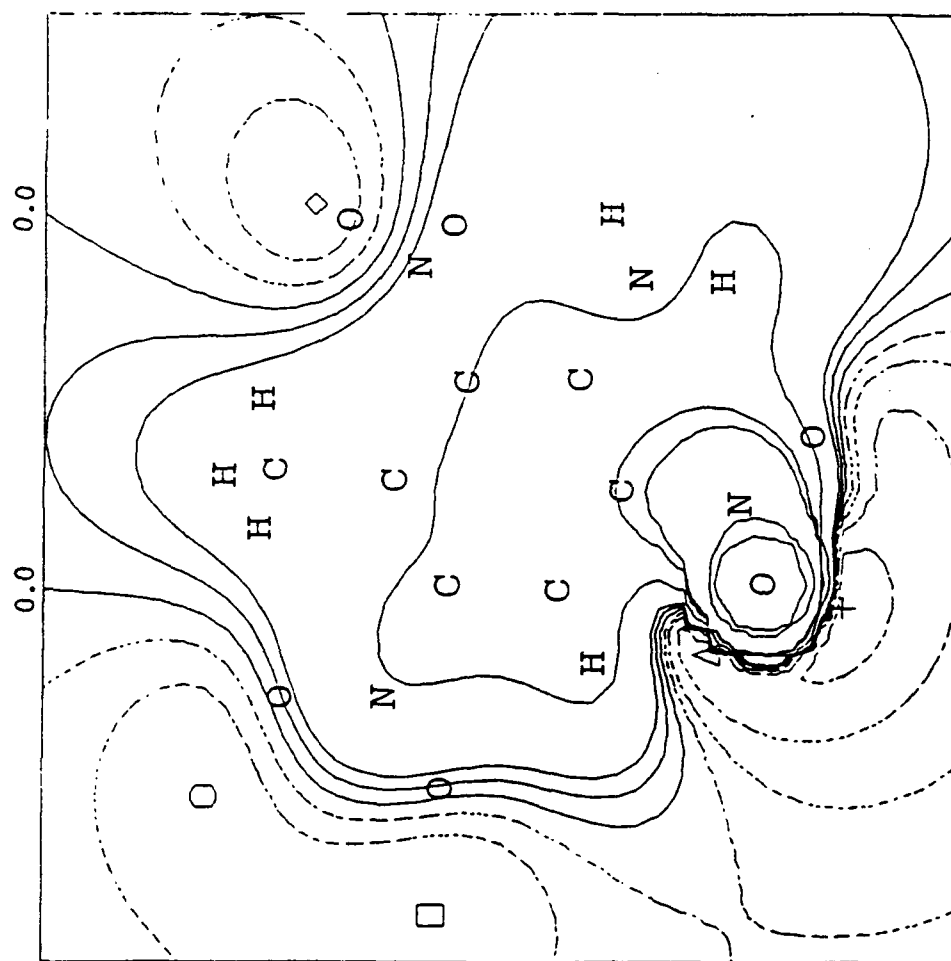


Figure G-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.100
 -12.550
 -6.275
 -3.138
 0.000
 3.138
 6.275
 25.100
 50.201
 62.751
 313.754
 627.509
 0.000



MINIMA	
□	-10.210
○	-9.193
△	-24.667
+	-41.359
◇	-9.708

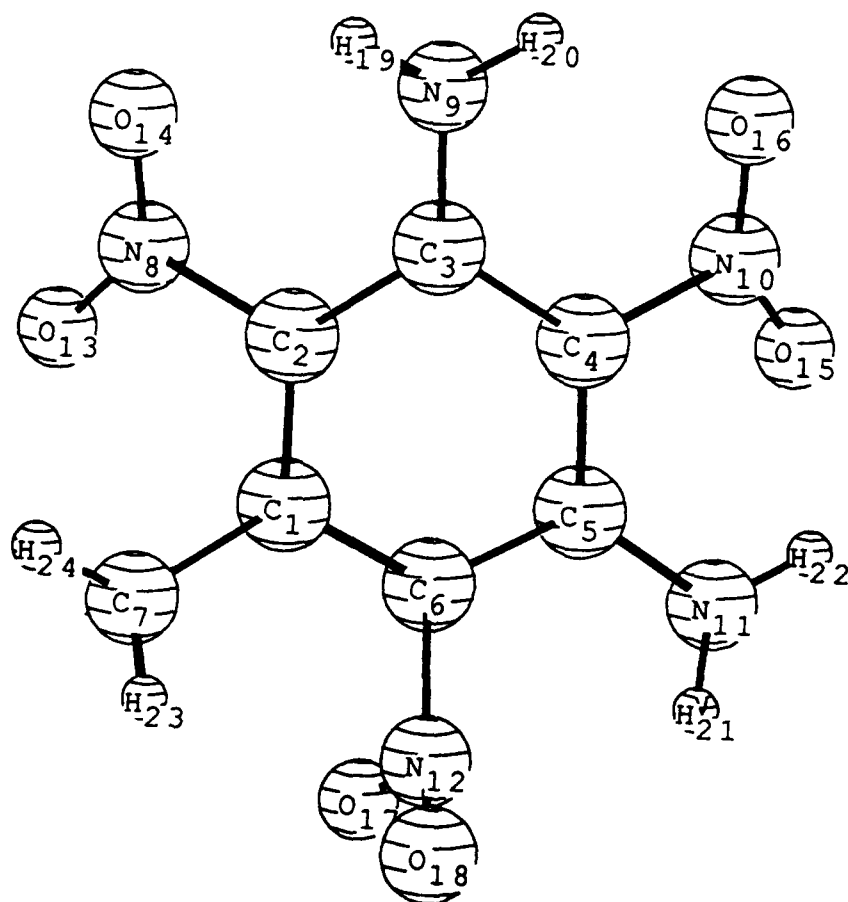
Figure G-2. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX H

3,5-DIAMINO-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H19-O14 (1.97 Å), H22-O15 (1.91 Å), H24-O13 (2.36 Å) and H20-O16 (1.89 Å).

The N8 and N10 nitro groups are rotated out of the mean plane of the benzene ring by approximately 34° and 22°, respectively. The N12 nitro group is almost perpendicular to the plane, being rotated by about 80°. The amine groups are approximately planar.



			Z-MATRIX (ANGSTROMS AND DEGREES)						
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.399500 (1)					
3	3	C	2	1.424227 (2)	1	123.518 (25)			
4	4	C	3	1.436338 (3)	2	116.441 (26)	1	5.613 (48)	0
5	5	C	4	1.415313 (4)	3	121.832 (27)	2	-3.717 (49)	0
6	6	C	5	1.408478 (5)	4	116.129 (28)	3	-1.141 (50)	0
7	7	C	1	1.488618 (6)	2	124.037 (29)	3	173.936 (51)	0
8	8	N	2	1.445386 (7)	3	118.672 (30)	4	-171.743 (52)	0
9	9	N	3	1.326379 (8)	4	121.753 (31)	5	179.278 (53)	0
10	10	N	4	1.434609 (9)	3	119.131 (32)	2	177.627 (54)	0
11	11	N	5	1.348888 (10)	4	124.060 (33)	3	-179.926 (55)	0
12	12	N	6	1.467081 (11)	5	116.345 (34)	4	-176.867 (56)	0
13	13	O	8	1.228633 (12)	2	118.018 (35)	3	144.720 (57)	0
14	14	O	8	1.232337 (13)	2	120.086 (36)	3	-34.210 (58)	0
15	15	O	10	1.241579 (14)	4	118.724 (37)	3	-159.360 (59)	0
16	16	O	10	1.230972 (15)	4	120.728 (38)	3	21.819 (60)	0
17	17	O	12	1.273003 (16)	6	116.635 (39)	5	-110.475 (61)	0
18	18	O	12	1.306374 (17)	6	114.235 (40)	5	98.241 (62)	0
19	19	H	9	0.852295 (18)	3	116.430 (41)	4	-177.948 (63)	0
20	20	H	9	0.910176 (19)	3	118.244 (42)	4	-6.893 (64)	0
21	21	H	11	0.892919 (20)	5	115.418 (43)	4	172.211 (65)	0
22	22	H	11	0.920404 (21)	5	117.933 (44)	4	0.104 (66)	0
23	23	H	7	0.915330 (22)	1	114.609 (45)	2	-153.018 (67)	0
24	24	H	7	0.922669 (23)	1	110.973 (46)	2	-29.739 (68)	0
25	25	H	7	0.882767 (24)	1	112.314 (47)	2	85.590 (69)	0

STOICHIOMETRY C7H7N5O6

SCF DONE: E(RHF) = -985.905123075 A.U. AFTER 44 CYCLES

EIGENVALUES -- -0.28717 0.13494 0.15325 0.16704 0.22261

Estimated ionization potential: 7.82 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.888064	0.112
2	C	5.978831	0.022
3	C	5.775979	0.224
4	C	5.987531	0.012
5	C	5.788101	0.212
6	C	5.967760	0.032
7	C	6.393238	-0.393
8	N	6.842391	0.158
9	N	7.543006	-0.543
10	N	6.840932	0.159
11	N	7.508429	-0.508
12	N	6.903556	0.096
13	O	8.193744	-0.194
14	O	8.225308	-0.225
15	O	8.216013	-0.216
16	O	8.211316	-0.211
17	O	8.160196	-0.160
18	O	8.180407	-0.180
19	H	0.699784	0.300
20	H	0.705469	0.295
21	H	0.734572	0.265
22	H	0.708944	0.291
23	H	0.855701	0.144
24	H	0.852741	0.147
25	H	0.837985	0.162

DIPOLE MOMENT (DEBYE): X= 1.4423 Y=-0.2507 Z= 0.1758 TOTAL= 1.4745

V-mid: N8-C2: 0.132
 N10-C4: 0.126
 N12-C6: 0.092

BOND ORDER: N8-C2: 1.30
 N10-C4: 1.33
 N12-C6: 1.25
 O13-N8: 1.90
 O14-N8: 1.88
 O15-N10: 1.84
 O16-N10: 1.89
 O17-N12: 1.71
 O18-N12: 1.52

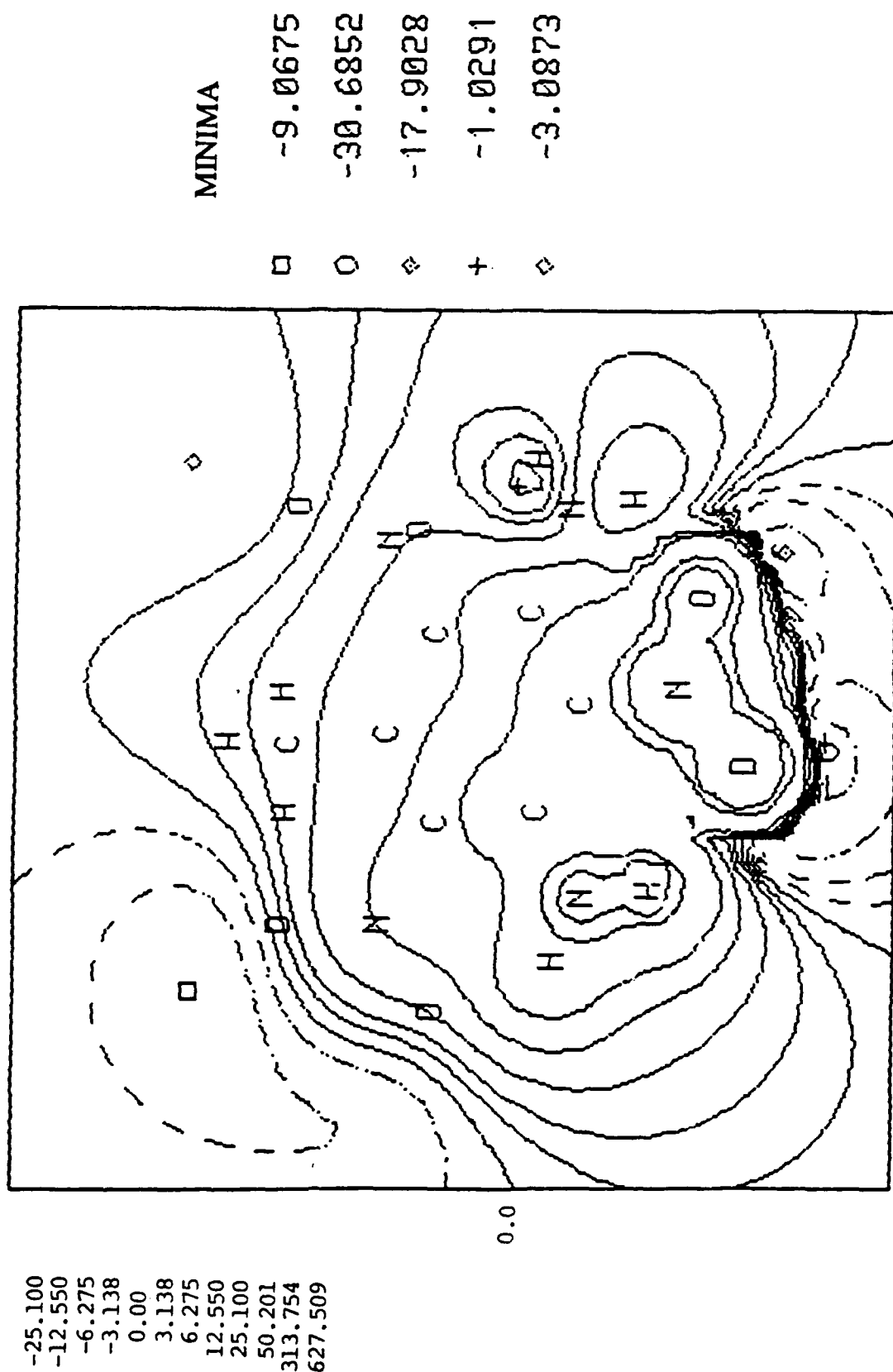


Figure H-1. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75 Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

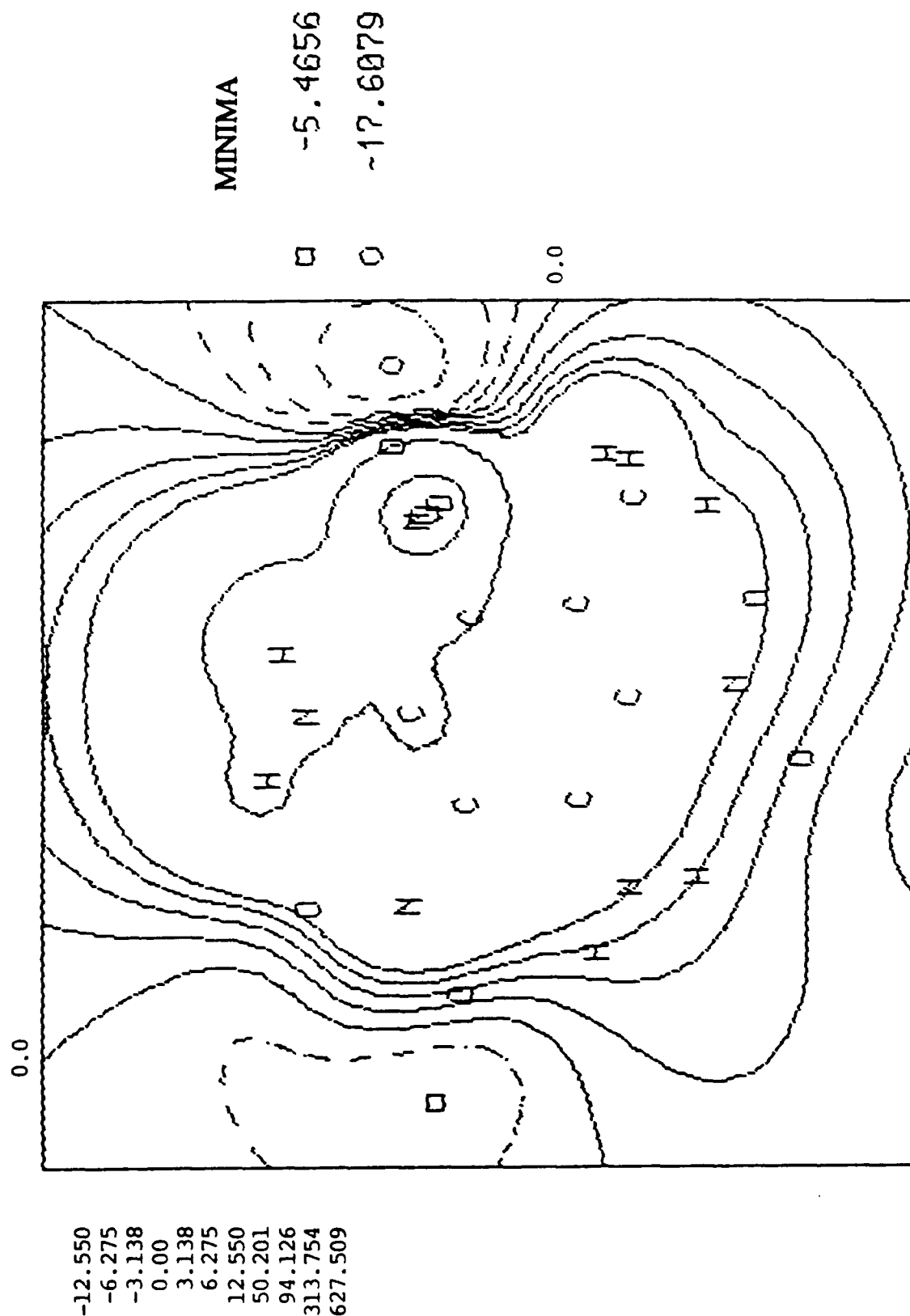
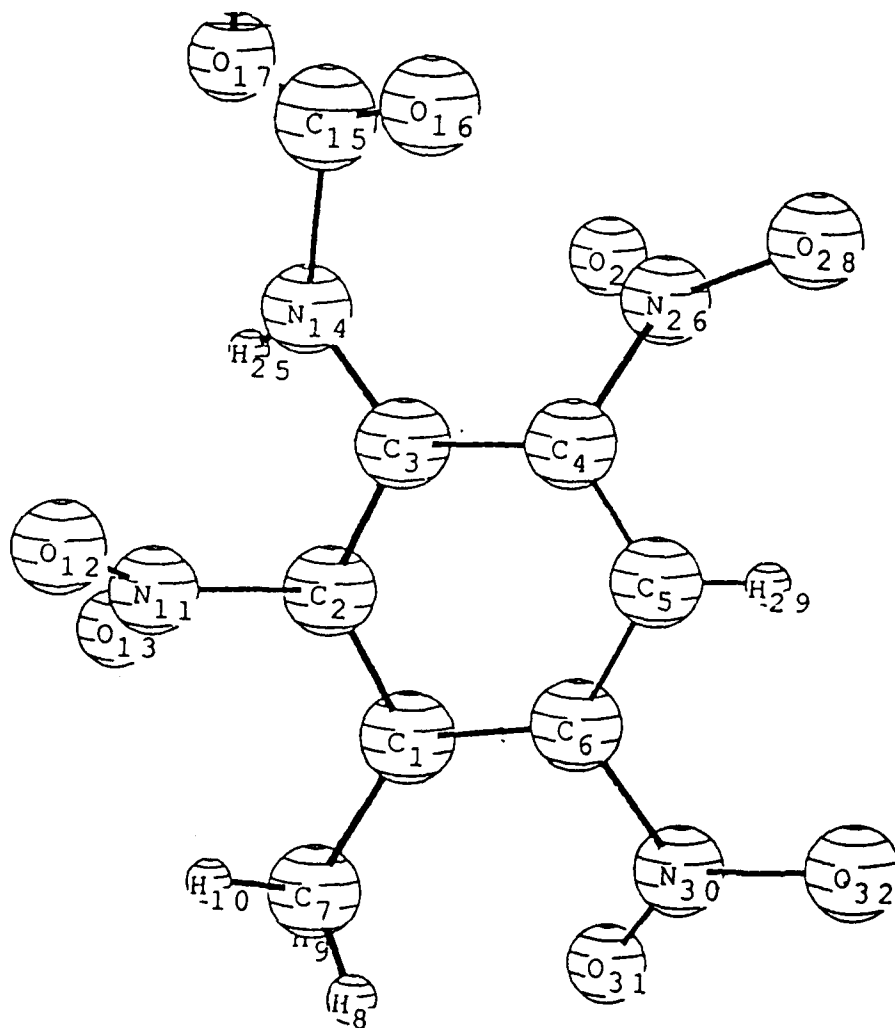


Figure H-2. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX I
N-CARBOETHOXY-2,4,6-TRINITRO-*m*-TOLUIDINE

The short distances between non-bonded hydrogens and oxygens are H19-O17 (1.93 Å), H20-O17 (1.91 Å), H25-O17 (2.33 Å) and H29-O32 (2.39 Å).

The N30 nitro group is rotated by approximately 26°, the N26 nitro group is rotated by approximately 43°, and the N11 nitro group is rotated by almost 80°.



The ethyl group bonded to O₁₇ is not shown for reasons of clarity.

Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.390250(1)					
3	3	C	2	1.391064(2)	1	126.771(32)			
4	4	C	3	1.390742(3)	2	115.503(33)	1	-4.433(62)	0
5	5	C	4	1.381592(4)	3	121.733(34)	2	0.756(63)	0
6	6	C	5	1.384425(5)	4	119.005(35)	3	3.511(64)	0
7	7	C	1	1.493449(6)	2	121.586(36)	3	-179.232(65)	0
8	8	H	7	0.967633(7)	1	115.478(37)	2	-139.662(66)	0
9	9	H	7	1.061986(8)	1	116.455(38)	2	101.196(67)	0
10	10	H	7	0.916674(9)	1	114.154(39)	2	-16.427(68)	0
11	11	N	2	1.482241(10)	3	115.743(40)	4	174.575(69)	0
12	12	O	11	1.212032(11)	2	117.007(41)	3	-77.802(70)	0
13	13	O	11	1.215249(12)	2	117.878(42)	3	102.172(71)	0
14	14	N	3	1.397079(13)	4	125.060(43)	5	-178.132(72)	0
15	15	C	14	1.361248(14)	3	122.077(44)	4	-44.150(73)	0
16	16	O	15	1.190292(15)	14	125.748(45)	3	-6.572(74)	0
17	17	O	15	1.346414(16)	14	105.923(46)	3	176.088(75)	0
18	18	C	17	1.447102(17)	15	116.375(47)	14	-177.238(76)	0
19	19	H	18	1.038544(18)	17	100.570(48)	15	-159.541(77)	0
20	20	H	18	0.924146(19)	17	109.974(49)	15	-55.325(78)	0
21	21	C	18	1.473267(20)	17	111.564(50)	15	80.220(79)	0
22	22	H	21	0.959974(21)	18	107.067(51)	17	53.634(80)	0
23	23	H	21	0.959906(22)	18	109.910(52)	17	-65.220(81)	0
24	24	H	21	0.959585(23)	18	111.414(53)	17	173.257(82)	0
25	25	H	14	0.945386(24)	3	116.967(54)	2	-50.333(83)	0
26	26	N	4	1.471524(25)	3	122.678(55)	2	176.140(84)	0
27	27	O	26	1.224059(26)	4	117.245(56)	3	-43.294(85)	0
28	28	O	26	1.226059(27)	4	117.577(57)	3	138.035(86)	0
29	29	H	5	0.929382(28)	4	121.749(58)	3	175.122(87)	0
30	30	N	6	1.485920(29)	1	121.348(59)	2	-177.203(88)	0
31	31	O	30	1.219037(30)	6	118.064(60)	1	27.472(89)	0
32	32	O	30	1.232587(31)	6	117.339(61)	1	-154.539(90)	0

STOICHIOMETRY C10H10N4O5

SCF DONE: E(RHF) = -1195.73406407

EIGENVALUES — -0.30684 0.12465 0.14400 0.18828 0.20432

Estimated ionization potential: 8.36 eV

Total atomic charges:

1

1	C	0.071515
2	C	0.005253
3	C	0.166048
4	C	0.102347
5	C	-2.066300
6	C	0.096009
7	C	-2.302283
8	H	0.129093
9	H	0.127210
10	H	0.125939
11	N	0.173171
12	C	-0.164355
13	C	-0.196279
14	N	0.406348
15	C	0.473059
16	C	-0.319455
17	C	-0.269170
18	C	-0.028449
19	H	0.096931
20	H	0.111969
21	C	-0.313272
22	H	0.114663
23	H	0.118637
24	H	0.113212
25	H	0.262822
26	N	0.175031
27	O	-0.198244
28	O	-0.176578
29	H	0.143709
30	N	0.167351
31	O	-0.190433
32	O	-0.193413

Sum of Mulliken charges= 0.00000

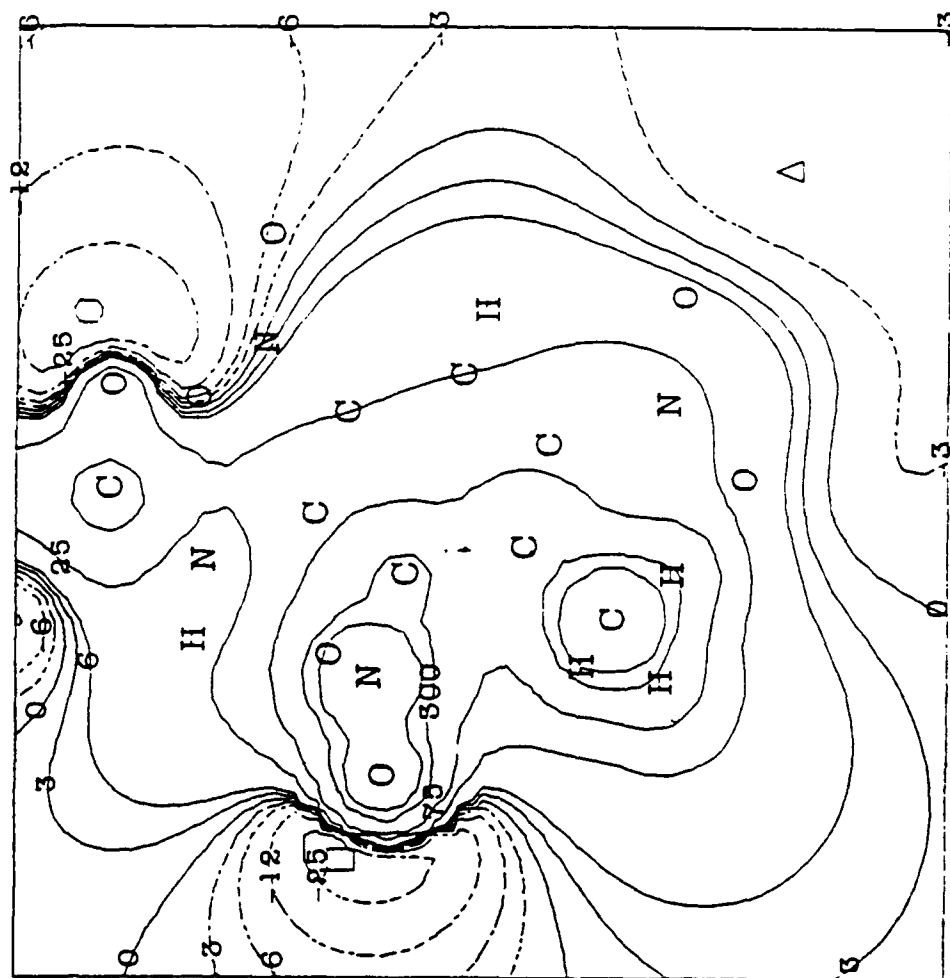
Dipole moment (Debye):

X=	-1.6558	Y=	1.1414	Z=	1.5154	Tot=	2.5182
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V-mid: N11-C2: 0.184
 N26-C4: 0.198
 N30-C6: 0.187

Bond Order: N11-C2: 1.21
 N26-C4: 1.24
 N30-C6: 1.20
 O12-N11: 1.98
 O13-N11: 1.96
 O27-N26: 1.92
 O28-N26: 1.91
 O31-N30: 1.94
 O32-N30: 1.88

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0

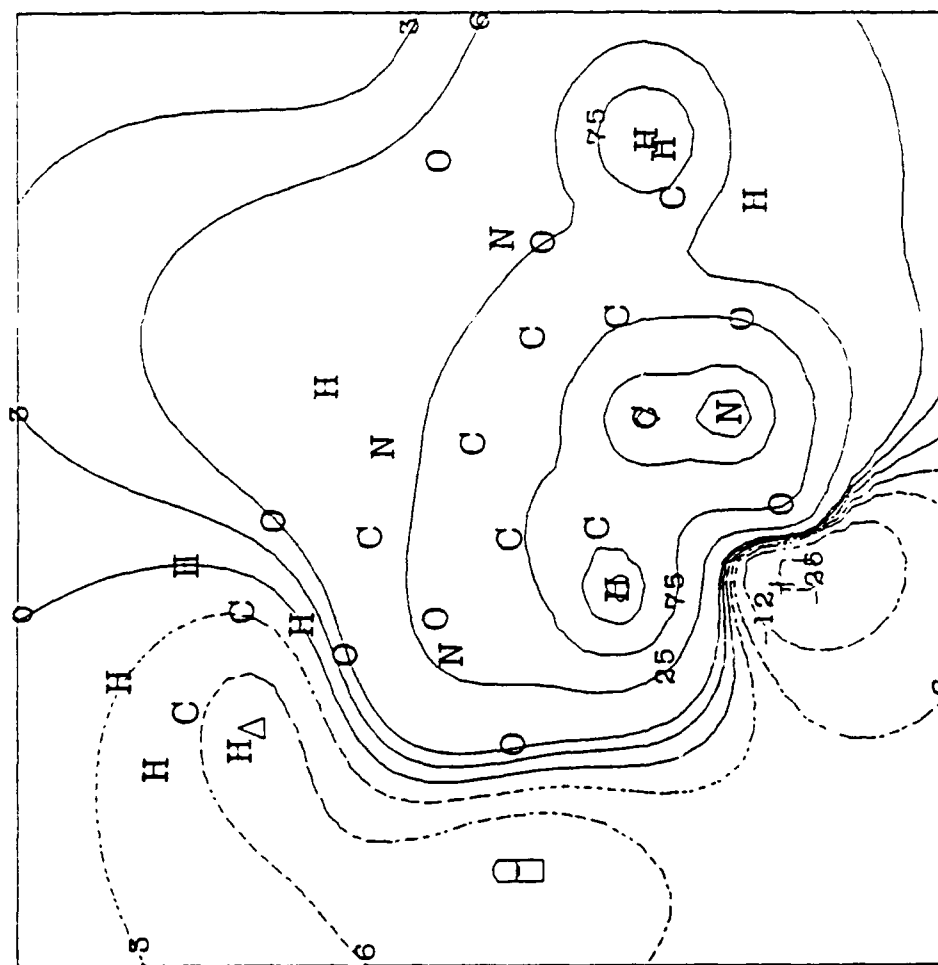


MINIMA

□ -37.920
○ -42.646
△ -5.064

Figure I-1. Calculated electrostatic potential, in kcal/mole, of N-carboethoxy-2,4,6-trinitro-m-toluidine, in the plane 1.75Å above the N30 nitro group located in the lower right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0



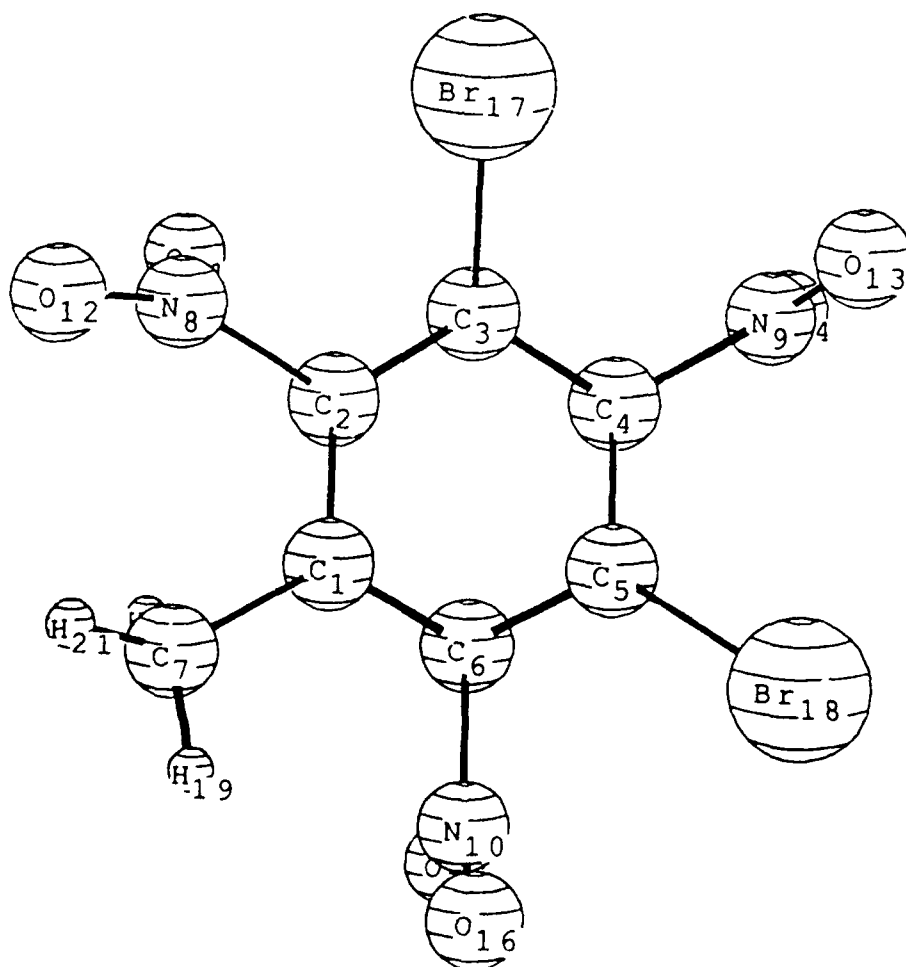
MINIMA
□ -8.635
○ -8.635
△ -7.122
+ -26.355

Figure I-2. Calculated electrostatic potential, in kcal/mole, of N-carboethoxy-2,4,6-trinitro-m-toluidine, in the plane 1.75Å above the N26 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX J
3,5-DIBROMO-2,4,6-TRINITROTOLUENE, #18

The only noticeable short distance between non-bonded hydrogens and oxygens is H21-O12 (2.50 Å).

The N8 and N10 nitro groups are rotated by approximately 62° and 80°, respectively. The N9 nitro group is roughly perpendicular to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C	1	1.370000(1)				
3	3	C	2	1.366230(2)	1	122.557(21)		
4	4	C	3	1.391364(3)	2	116.727(22)	1	1.580(40)
5	5	C	4	1.384690(4)	3	121.696(23)	2	-2.381(41)
6	6	C	5	1.356721(5)	4	117.881(24)	3	3.198(42)
7	7	C	1	1.499745(6)	2	120.350(25)	3	179.066(43)
8	8	N	2	1.507550(7)	3	116.858(26)	4	177.670(44)
9	9	N	4	1.497292(8)	5	118.760(27)	6	-178.324(45)
10	10	N	6	1.498023(9)	5	118.516(28)	4	-179.612(46)
11	11	O	8	1.215329(10)	2	116.760(29)	1	-116.703(47)
12	12	O	8	1.207687(11)	2	117.680(30)	1	60.430(48)
13	13	O	9	1.169336(12)	4	117.809(31)	3	90.462(49)
14	14	O	9	1.196739(13)	4	116.397(32)	3	-86.695(50)
15	15	O	10	1.212542(14)	6	116.156(33)	5	-101.694(51)
16	16	O	10	1.154568(15)	6	118.205(34)	5	81.236(52)
17	17	Br	3	1.868548(16)	4	119.748(35)	5	177.402(53)
18	18	Br	5	1.866427(17)	4	121.248(36)	3	-177.609(54)
19	19	H	7	0.999707(18)	1	109.529(37)	2	179.714(55)
20	20	H	7	0.992240(19)	1	109.952(38)	2	59.233(56)
21	21	H	7	1.010376(20)	1	109.447(39)	2	-60.330(57)

STOICHIOMETRY C7H3Br2N3O6

SCF DONE: E(RHF) = -5992.86404190

Alpha eigenvalues — -0.33079 -0.32411 0.14114 0.15325 0.19239

Estimated ionization potential: 8.83 ev

Total atomic charges:

1
 1 C 0.062394
 2 C 0.085894
 3 C -0.030675
 4 C 0.092229
 5 C -0.032007
 6 C 0.083762
 7 C -0.272475
 8 N 0.181223
 9 N 0.203254
 10 N 0.204171
 11 O -0.182988
 12 O -0.187541
 13 O -0.185329
 14 O -0.194150
 15 O -0.204145
 16 O -0.182049
 17 Br 0.104333
 18 Br 0.098127
 19 H 0.112404
 20 H 0.118445
 21 H 0.125125

Dipole moment (Debye):

X= 0.0680 Y= 1.2263 Z= -0.2630 Tot= 1.2560

Bond Order: C2-N8: 1.15

C4-N9: 1.17

C6-N10: 1.17

N8-O11: 1.96

N8-O12: 2.00

N9-O13: 2.20

N9-O14: 2.05

N10-O15: 1.97

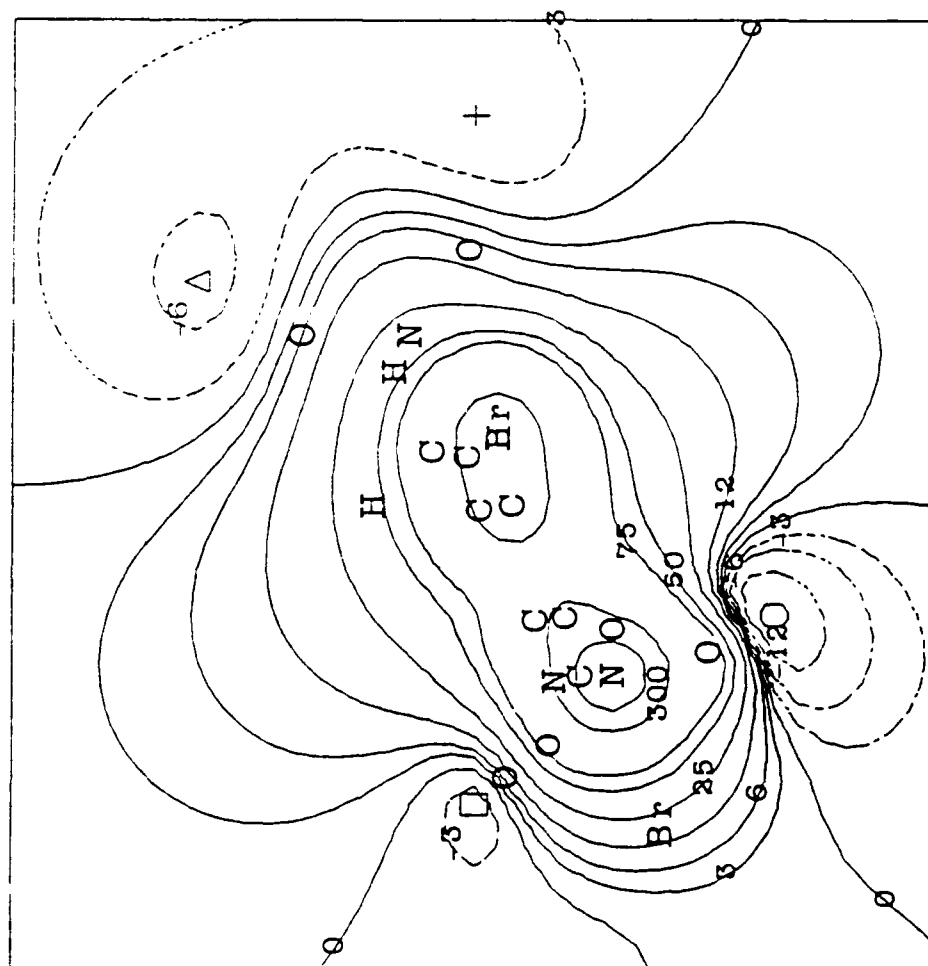
N10-O16: 2.28

V-mid: C2-N8: 0.187

C4-N9: 0.209

C6-N10: 0.203

-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
300.0
600.0

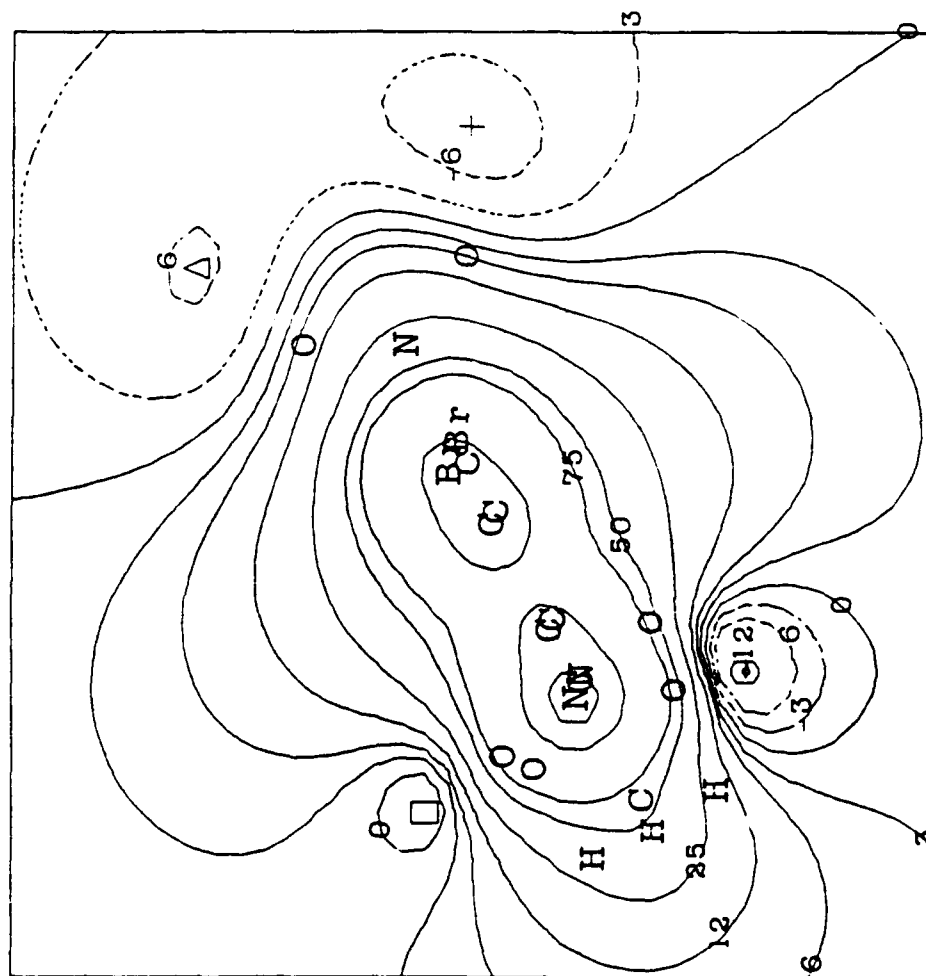


MINIMA

□ -4.3
○ -20.7
△ -6.8
+ -5.0

Figure J-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
300.0
600.0



MINIMA

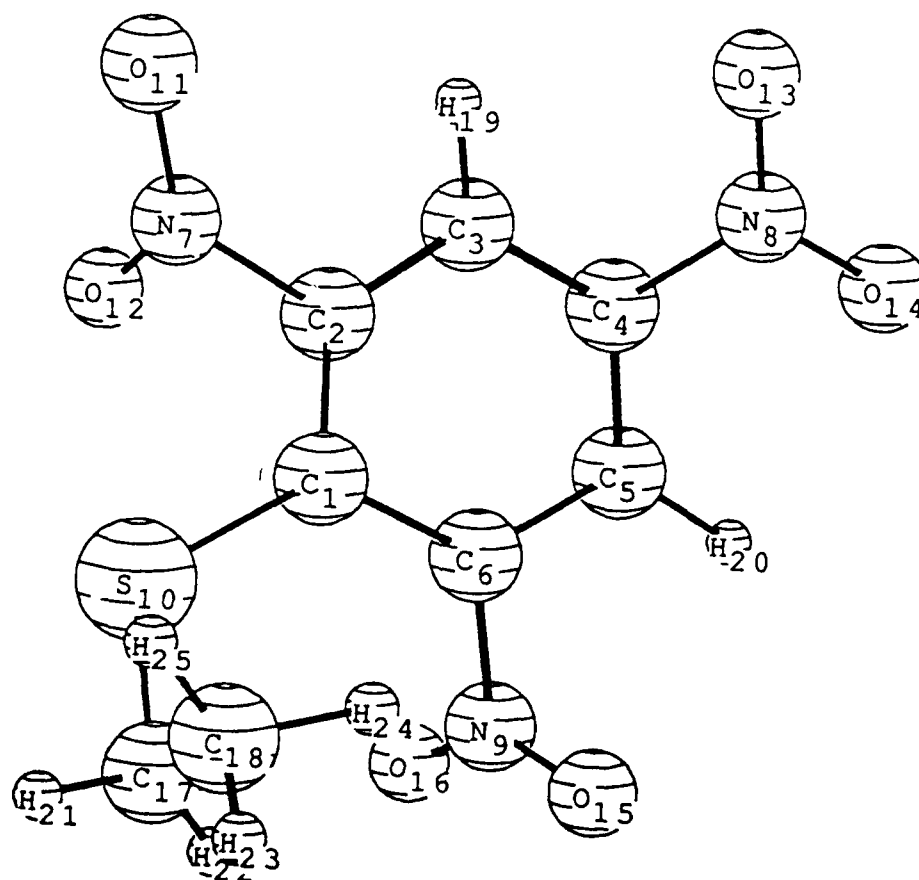
□ -2.1
○ -12.5
△ -6.3
+ -7.2

Figure J-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dibromo-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX K ETHYL PICRYL SULFIDE

The short distances between non-bonded hydrogens and oxygens are H20-O14 (2.50 Å), H20-O15 (2.46 Å), H19-O11 (2.44 Å) and H19-O13 (2.51 Å).

The N7, N8 and N9 nitro groups are rotated out of the mean plane of the benzene ring by approximately 38°, 18°, and 45°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C		1.375900(1)				
3	3	C	2	1.376557(2)	1	124.918(25)		
4	4	C	3	1.382829(3)	2	118.200(26)	1	2.681(48) 0
5	5	C	4	1.398791(4)	3	121.456(27)	2	-0.590(49) 0
6	6	C	5	1.380410(5)	4	117.821(28)	3	0.481(50) 0
7	7	N	2	1.489709(6)	3	115.593(29)	4	178.934(51) 0
8	8	N	4	1.457060(7)	5	118.259(30)	6	177.848(52) 0
9	9	N	6	1.454312(8)	5	114.988(31)	4	175.943(53) 0
10	10	S	1	1.768547(9)	2	120.736(32)	3	172.875(54) 0
11	11	O	7	1.204119(10)	2	117.786(33)	3	-37.560(55) 0
12	12	O	7	1.217904(11)	2	116.236(34)	3	139.586(56) 0
13	13	O	8	1.222714(12)	4	117.912(35)	5	-164.154(57) 0
14	14	O	8	1.230870(13)	4	117.508(36)	5	18.345(58) 0
15	15	O	9	1.217474(14)	6	117.764(37)	5	44.712(59) 0
16	16	O	9	1.227813(15)	6	117.917(38)	5	-131.235(60) 0
17	17	C	10	1.835985(16)	1	104.995(39)	2	-139.082(61) 0
18	18	C	17	1.504611(17)	10	112.827(40)	1	52.836(62) 0
19	19	H	3	1.035447(18)	4	123.308(41)	5	171.276(63) 0
20	20	H	5	1.094535(19)	4	124.362(42)	3	-177.750(64) 0
21	21	H	17	0.932937(20)	10	97.287(43)	1	161.355(65) 0
22	22	H	17	1.002419(21)	10	98.658(44)	1	-76.501(66) 0
23	23	H	18	0.820296(22)	17	103.954(45)	10	-179.864(67) 0
24	24	H	18	1.070622(23)	17	107.139(46)	10	-75.941(68) 0
25	25	H	18	0.903100(24)	17	103.590(47)	10	49.199(69) 0

STOICHIOMETRY C5H7N3O6S

SCF DONE: E(RHF) = -1311.18935285 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.31944 -0.31341 -0.30798 -0.29044 0.11847

Estimated ionization potential: 7.91 ev

Total atomic charges:

1
 1 C -0.062009
 2 C 0.081244
 3 C -0.037111
 4 C 0.087693
 5 C -0.021925
 6 C 0.078326
 7 N 0.178837
 8 N 0.165323
 9 N 0.159745
 10 S 0.245111
 11 O -0.196161
 12 O -0.192559
 13 O -0.190670
 14 O -0.195923
 15 O -0.190331
 16 O -0.195321
 17 C -0.230302
 18 C -0.347789
 19 H 0.140349
 20 H 0.134270
 21 H 0.114158
 22 H 0.111445
 23 H 0.141620
 24 H 0.097764
 25 H 0.124216

Dipole moment (Debye):

X= -1.7950 Y= -0.5715 Z= 0.9981 Tot= 2.1319

V-mid: C2-N7: 0.185

C4-N8: 0.164

C6-N9: 0.173

Bond Order: C2-N7: 1.19

C4-N8: 1.27

C6-N9: 1.28

N7-O11: 2.02

N7-O12: 1.95

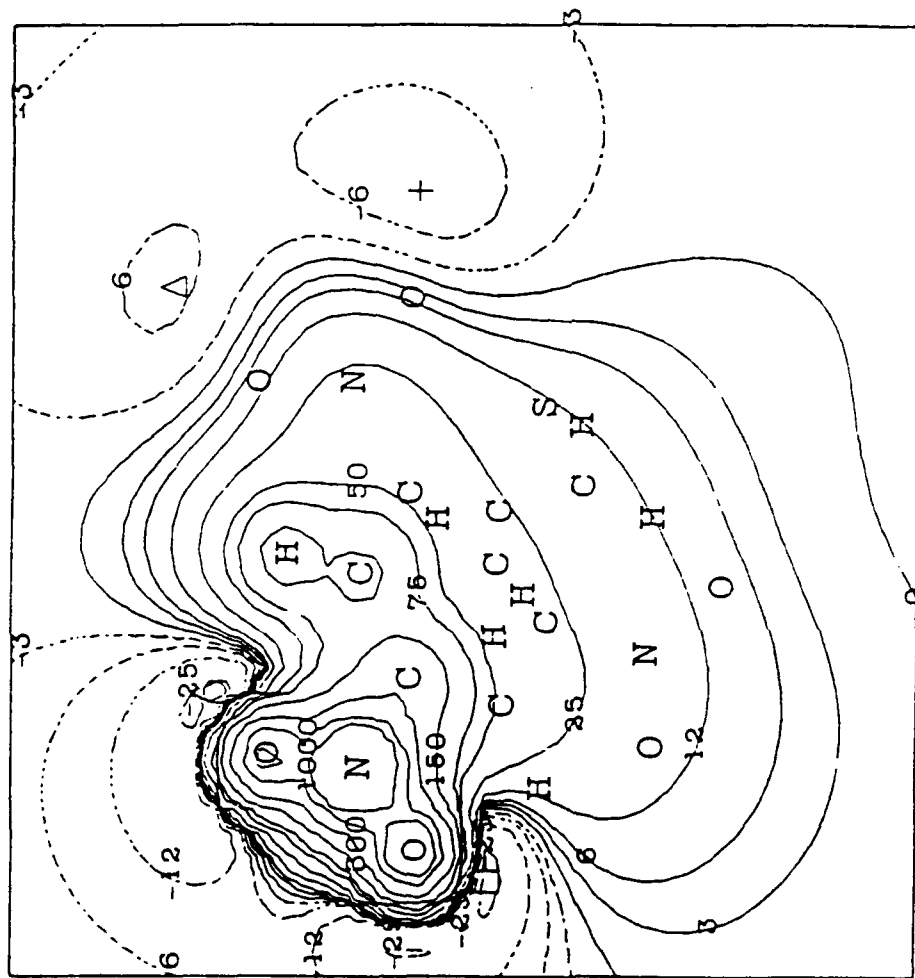
N8-O13: 1.92

N8-O14: 1.89

N9-O15: 1.95

N9-O16: 1.90

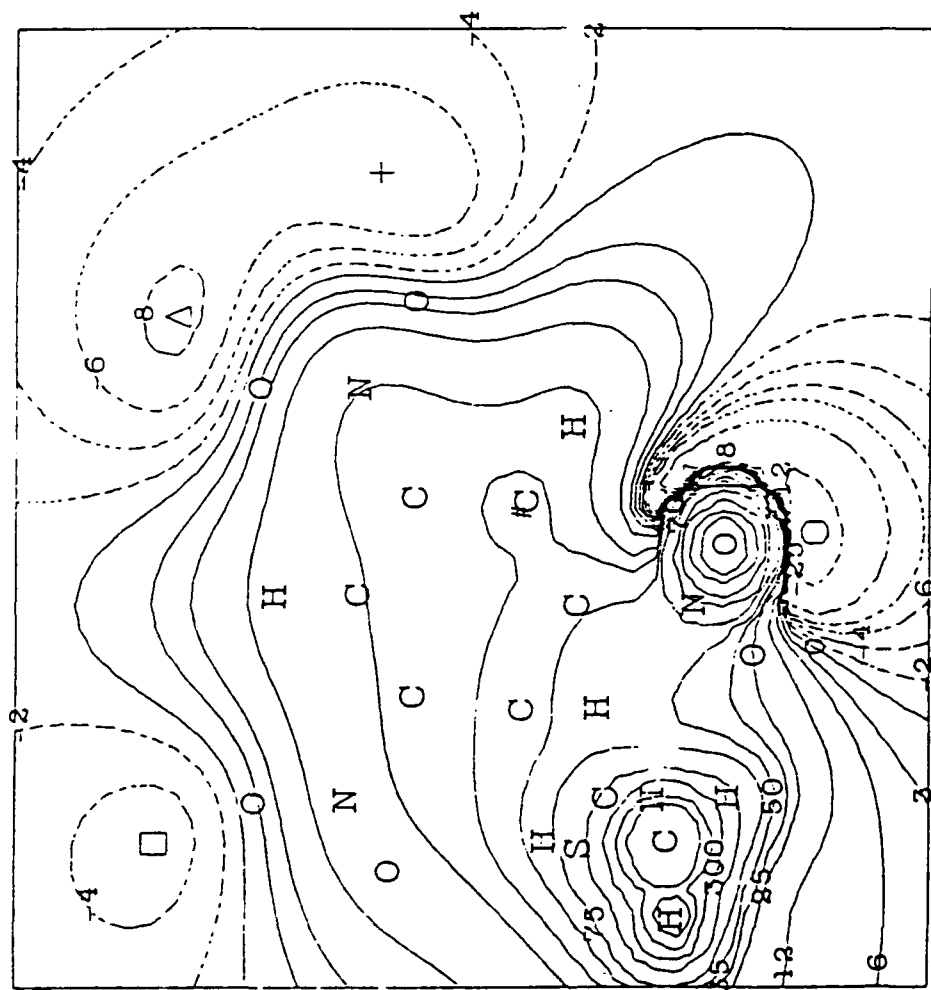
-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA
□ -29.6
○ -29.4
△ -6.4
+ -7.8

Figure K-1. Calculated electrostatic potential, in kcal/mole, of ethyl picryl sulfide, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-8.0
-6.0
-4.0
-2.0
0.0
3.0
6.0
12.0
25.0
35.0
50.0
75.0
150.0
300.0
600.0
1000.0

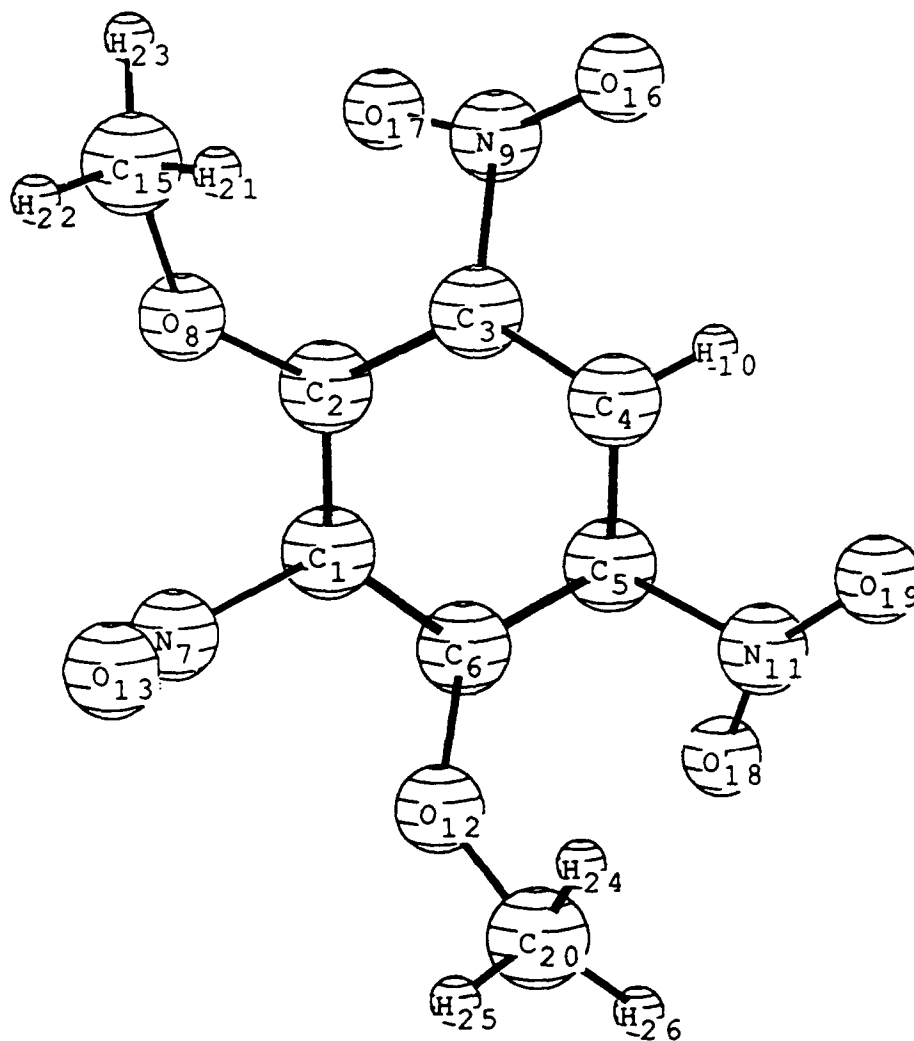


MINIMA
□ -4.9
○ -37.8
△ -8.5
+ -7.9
MAXIMA
+37.7

Figure K-2. Calculated electrostatic potential, in kcal/mole, of ethyl picryl sulfide, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX L
1,3-DIMETHOXY-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H10-O16 (2.40 Å), H10-O19 (2.40 Å), H23-O17 (2.40 Å) and H16-O18 (2.40 Å). Nitro groups N7, N9 and N11 are rotated out of the plane by approximately 87°, 28° and 24°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.380400 (1)					
3	3	C	2	1.396859 (2)	1	115.604 (26)			
4	4	C	3	1.374392 (3)	2	120.903 (27)	1	-0.300 (50)	0
5	5	C	4	1.374392 (4)	3	120.965 (28)	2	1.583 (51)	0
6	6	C	5	1.396707 (5)	4	120.903 (29)	3	-1.577 (52)	0
7	7	N	1	1.477729 (6)	2	116.814 (30)	3	171.627 (53)	0
8	8	O	2	1.348742 (7)	3	127.817 (31)	4	177.893 (54)	0
9	9	N	3	1.472888 (8)	4	116.550 (32)	5	-173.595 (55)	0
10	10	H	4	0.957800 (9)	5	119.491 (33)	6	-178.910 (56)	0
11	11	N	5	1.472798 (10)	6	122.351 (34)	1	-174.561 (57)	0
12	12	O	6	1.348835 (11)	1	116.545 (35)	2	179.456 (58)	0
13	13	O	7	1.201446 (12)	1	117.779 (36)	2	-86.685 (59)	0
14	14	O	7	1.196814 (13)	1	118.545 (37)	2	93.320 (60)	0
15	15	C	8	1.453946 (14)	2	118.793 (38)	3	-52.068 (61)	0
16	16	O	9	1.218047 (15)	3	116.743 (39)	4	-27.682 (62)	0
17	17	O	9	1.208641 (16)	3	118.554 (40)	4	150.656 (63)	0
18	18	O	11	1.208165 (17)	5	118.594 (41)	6	24.374 (64)	0
19	19	O	11	1.219471 (18)	5	116.707 (42)	6	-157.172 (65)	0
20	20	C	12	1.454637 (19)	6	118.815 (43)	1	-126.127 (66)	0
21	21	H	15	0.959584 (20)	8	110.128 (44)	2	-15.097 (67)	0
22	22	H	15	0.835747 (21)	7	102.071 (45)	2	-131.703 (68)	0
23	23	H	15	1.068769 (22)	8	106.925 (46)	2	107.973 (69)	0
24	24	H	20	0.959585 (23)	12	110.102 (47)	6	15.120 (70)	0
25	25	H	20	0.835635 (24)	12	102.070 (48)	6	131.718 (71)	0
26	26	H	20	1.068860 (25)	12	106.978 (49)	6	-107.899 (72)	0

STOICHIOMETRY C8H7N3O8

SCF DONE: E(RHF) = -1064.13065218 A.U. AFTER 27 CYCLES

EIGENVALUES -0.31717 0.12601 0.14363 0.20984 0.21092 0.24237

Estimated ionization potential: 8.66 ev

TOTAL ATOMIC CHARGES.

		1	Net charge
1	C	5.940192	0.060
2	C	5.809986	0.110
3	C	5.939638	0.060
4	C	6.051206	-0.051
5	C	5.939640	0.060
6	C	5.810025	0.190
7	N	6.801851	0.198
8	O	8.225877	-0.226
9	N	6.822849	0.177
10	H	0.852770	0.147
11	N	6.823226	0.177
12	O	8.225815	-0.226
13	O	8.208906	-0.209
14	O	8.183193	-0.183
15	C	6.187587	-0.188
16	O	8.197942	-0.198
17	O	8.196408	-0.196
18	O	8.195929	-0.196
19	O	8.198151	-0.198
20	C	6.187626	-0.188
21	H	0.881395	0.119
22	H	0.853922	0.146
23	H	0.865290	0.135
24	H	0.881356	0.119
25	H	0.853904	0.146
26	H	0.865314	0.135

DIPOLE MOMENT (DEBYE): X= 0.2854 Y=-2.4370 Z= 0.1182 TOTAL= 2.4565

V-mid: N7-C1: 0.185
 N9-C3: 0.170
 N11-C5: 0.170

Bond Order: N7-C1: 1.22
 N9-C3: 1.23
 N11-C5: 1.23
 O13-N7: 2.03
 O14-N7: 2.05
 O16-N9: 1.95
 O17-N9: 1.99
 O18-N11: 2.00
 O19-N11: 1.94

0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 62.751
 313.754
 627.509
 0.000

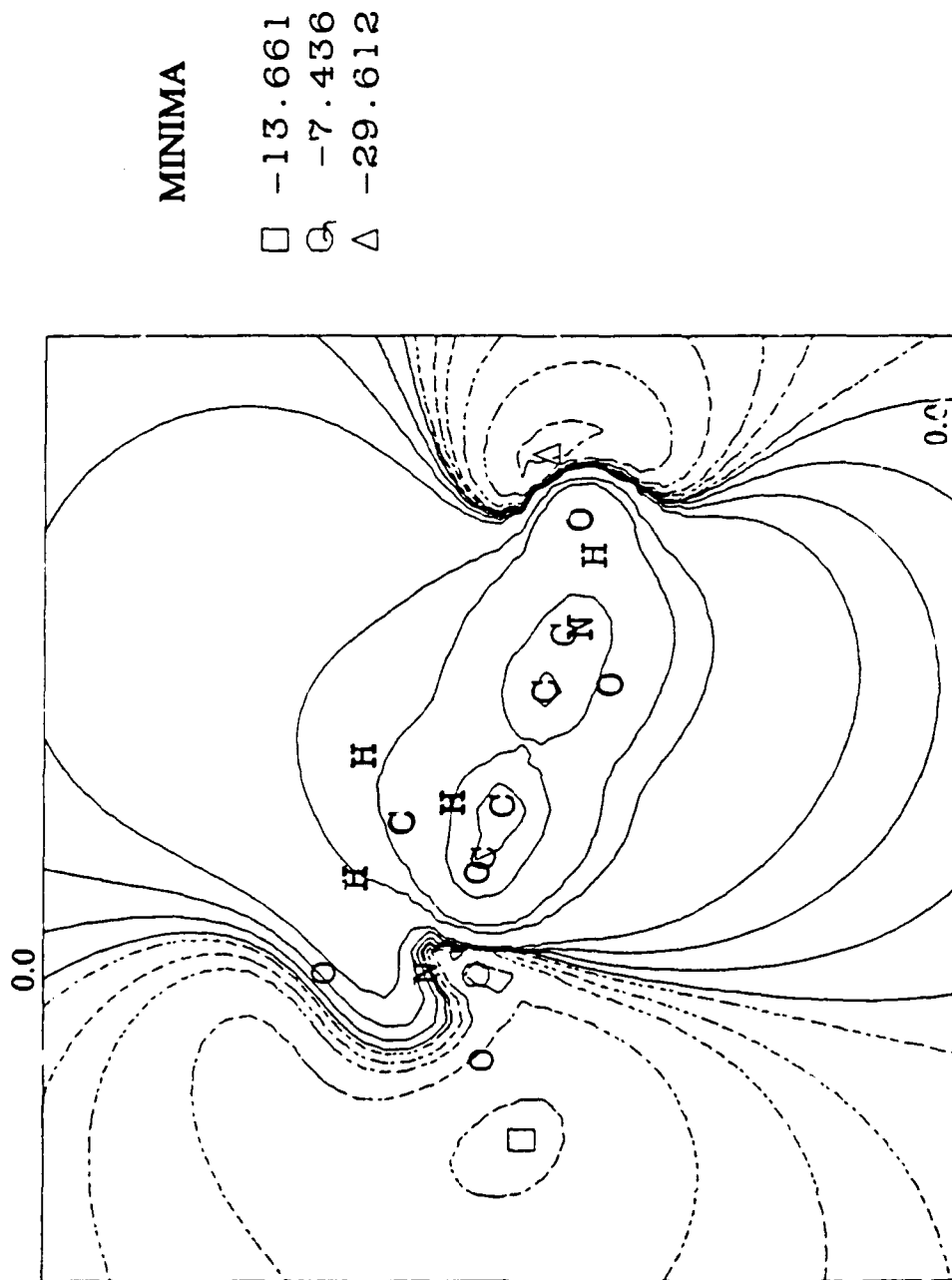


Figure L-1. Calculated electrostatic potential, in kcal/mole, of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75 Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 62.751
 313.754
 627.509
 0.000

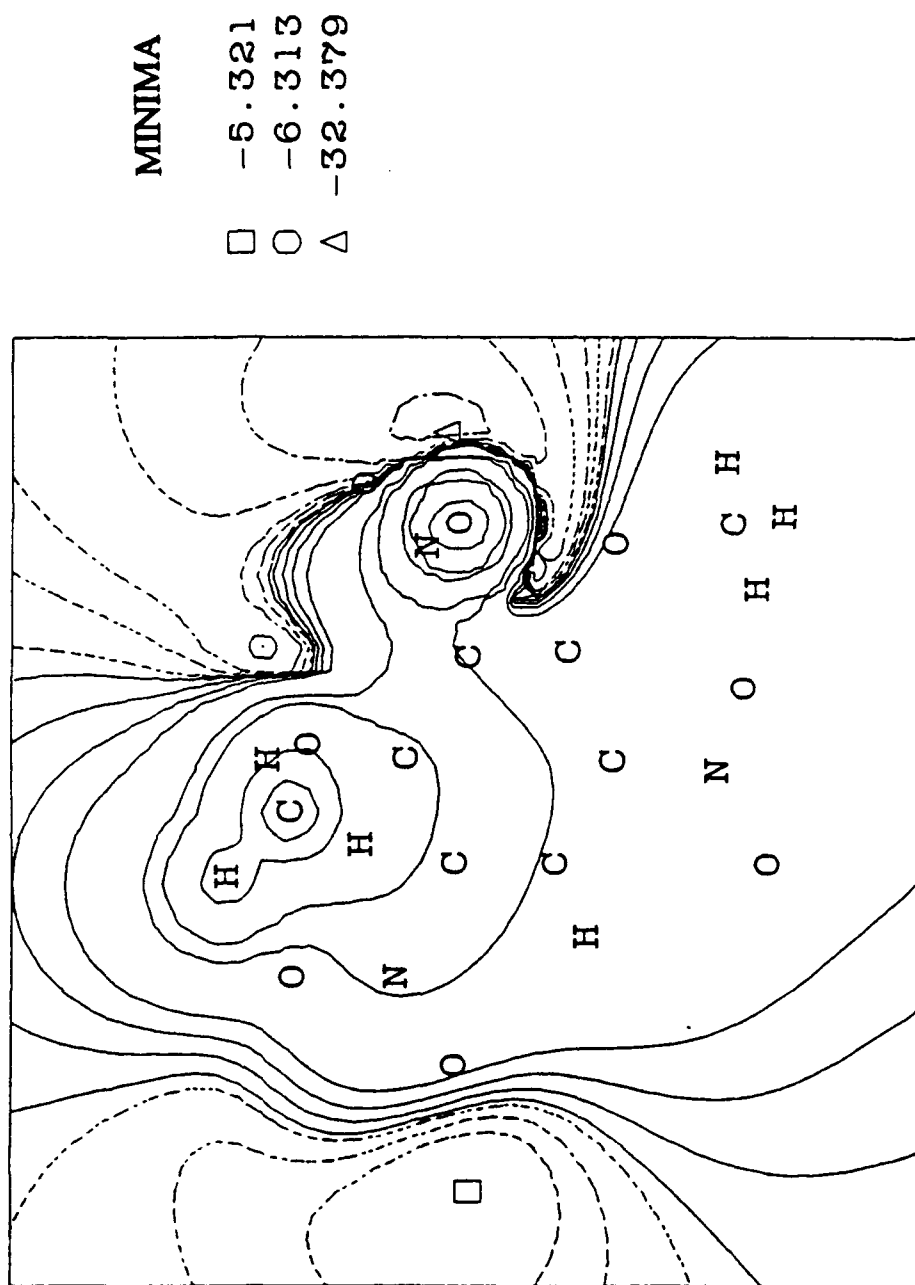
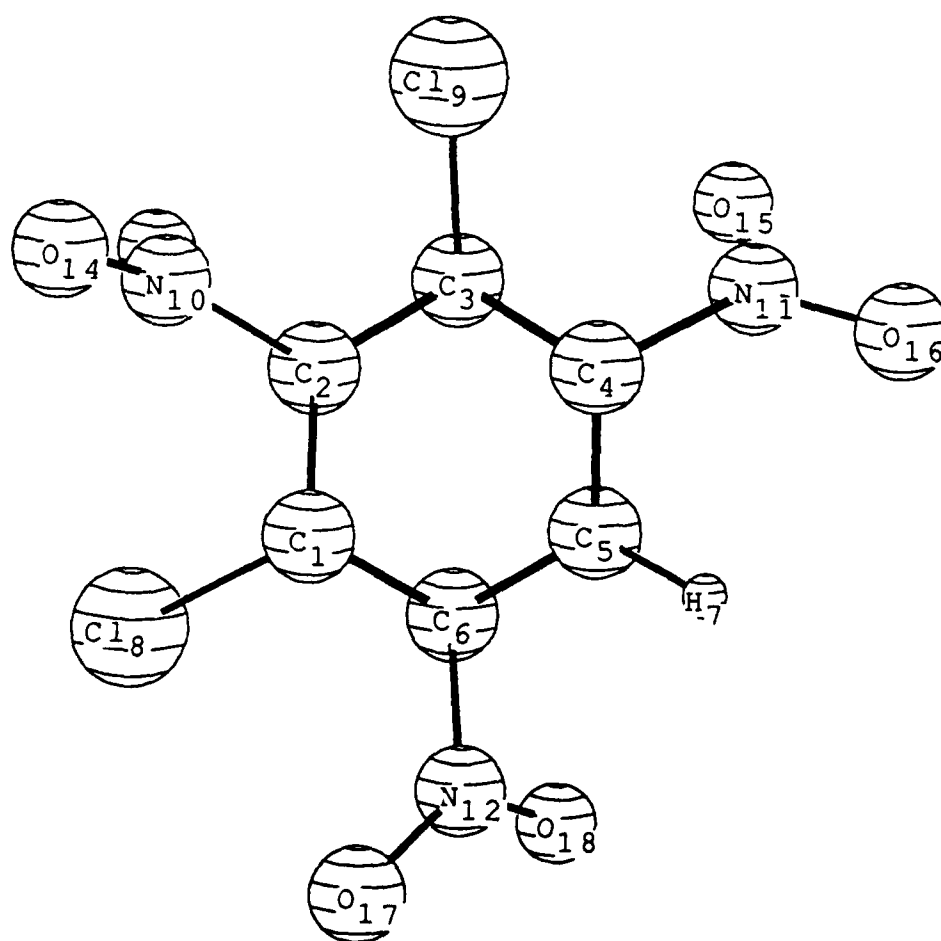


Figure L-2. Calculated electrostatic potential, in kcal/mole, of 1,3-dimethoxy-2,4,6-trinitrobenzene, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contour is indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX M
1,3-DICHLORO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are O18-H7 (2.48 Å) and O16-H7 (2.50 Å).

The N11 and N12 nitro groups are rotated out of the plane by about 37°, while the N10 nitro group is rotated by approximately 75°.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.407000 (1)					
3	3	C	2	1.407000 (2)	1	122.700 (18)			
4	4	C	3	1.371000 (3)	2	116.900 (19)	1	-0.100 (34)	0
5	5	C	4	1.378000 (4)	3	121.600 (20)	2	0.200 (35)	0
6	6	C	5	1.378000 (5)	4	120.200 (21)	3	-0.100 (36)	0
7	7	H	5	1.059000 (6)	4	119.900 (22)	3	179.900 (37)	0
8	8	Cl	1	1.690000 (7)	2	118.300 (23)	3	-177.800 (38)	0
9	9	Cl	3	1.690000 (8)	4	124.800 (24)	5	177.700 (39)	0
10	10	N	2	1.447000 (9)	3	118.600 (25)	9	2.200 (40)	0
11	11	N	4	1.467000 (10)	5	116.900 (26)	7	2.200 (41)	0
12	12	N	6	1.467000 (11)	5	116.900 (27)	4	-177.800 (42)	0
13	13	O	10	1.206000 (12)	2	117.300 (28)	3	74.800 (43)	0
14	14	O	10	1.206000 (13)	2	117.300 (29)	3	-105.200 (44)	0
15	15	O	11	1.224000 (14)	4	117.900 (30)	3	-35.300 (45)	0
16	16	O	11	1.217000 (15)	4	117.200 (31)	5	-37.800 (46)	0
17	17	O	12	1.224000 (16)	6	117.900 (32)	1	-37.800 (47)	0
18	18	O	12	1.217000 (17)	6	117.200 (33)	5	-35.300 (48)	0

STOICHIOMETRY C6HCL2N3O6

E= -1751.88563620

EIGENVALUES — -0.38138 -0.38065 -0.32917 -0.32775 -0.32741

Estimated ionization potential: 8.9 ev

TOTAL ATOMIC CHARGES.

	1	<u>Net Charges</u>
1 C	5.945256	+0.05
2 C	5.881767	+0.12
3 C	5.945048	+0.05
4 C	5.897801	+0.10
5 C	6.021674	-0.02
6 C	5.897935	+0.10
7 H	0.853928	+0.15
8 Cl	17.012369	-0.01
9 Cl	17.011478	-0.01
10 N	6.818918	+0.18
11 N	6.825640	+0.17
12 N	6.825625	+0.17
13 O	8.175416	-0.18
14 O	8.175321	-0.18
15 O	8.172938	-0.17
16 O	8.182942	-0.18
17 O	8.172556	-0.17
18 O	8.183389	-0.18

DIPOLE MOMENT (DEBYE): X= 0.9514 Y= 0.0777 Z=-0.5464 TOTAL= 1.0999

V_{mid}: C₂-N₁₀: 0.219
 C₄-N₁₁: 0.200
 C₆-N₁₂: 0.199

Bond Orders: C₂-N₁₀: 1.31
 C₄-N₁₁: 1.25
 C₆-N₁₂: 1.25
 N₁₀-O₁₃: 2.17
 N₁₀-O₁₄: 2.17
 N₁₁-O₁₅: 2.07
 N₁₁-O₁₆: 2.11
 N₁₂-O₁₇: 2.07
 N₁₂-O₁₈: 2.11

□	-15.763
○	-21.561
△	-21.975
+	-21.674
◇	-29.681

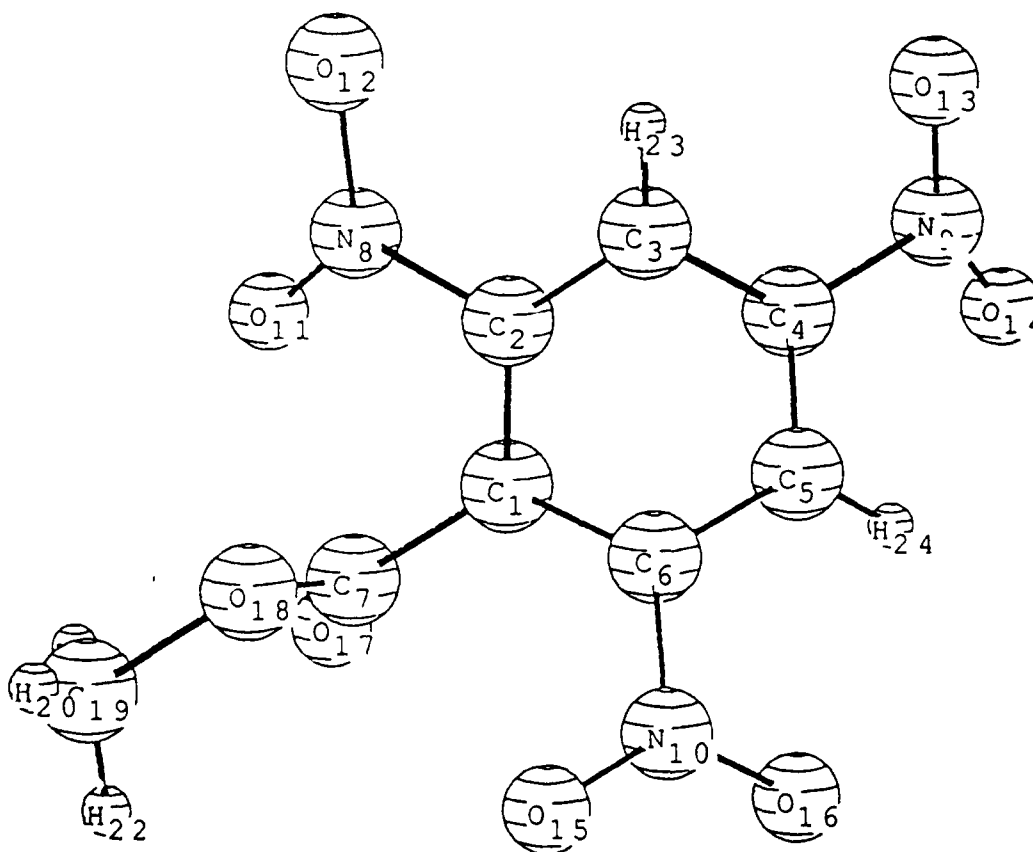
$$= +43,844$$

Figure M-1. Calculated electrostatic potential, in kcal/mole, of 1,3-dichloro-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX N
METHYL 2,4,6-TRINITROBENZOATE

The short distances between non-bonded hydrogens and oxygens are H24-O16 (2.39 Å), H24-O14 (2.49 Å), H23-O12 (2.51 Å), and H23-O13 (2.46 Å).

The N8, N9 and N10 nitro groups are rotated out of the mean plane of the benzene ring by about 30°, 19° and 11°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA
1	1	C						
2	2	C	1	1.399000 (1)				
3	3	C	2	1.369201 (2)	1	123.039 (24)		
4	4	C	3	1.367792 (3)	2	118.034 (25)	1	3.951 (46) 0
5	5	C	4	1.381531 (4)	3	122.096 (26)	2	-5.419 (47) 0
6	6	C	5	1.373809 (5)	4	117.508 (27)	3	2.053 (48) 0
7	7	C	1	1.506101 (6)	2	121.789 (28)	3	-174.205 (49) 0
8	8	N	2	1.473057 (7)	3	117.045 (29)	4	-175.495 (50) 0
9	9	N	4	1.468854 (8)	3	119.287 (30)	2	176.619 (51) 0
10	10	N	6	1.469922 (9)	5	116.809 (31)	4	-174.204 (52) 0
11	11	O	8	1.219024 (10)	2	117.687 (32)	3	146.477 (53) 0
12	12	O	8	1.200891 (11)	2	118.570 (33)	3	-30.182 (54) 0
13	13	O	9	1.204490 (12)	4	117.840 (34)	3	18.816 (55) 0
14	14	O	9	1.212250 (13)	4	117.908 (35)	3	-160.143 (56) 0
15	15	O	10	1.215152 (14)	6	118.306 (36)	5	167.609 (57) 0
16	16	O	10	1.202680 (15)	6	118.492 (37)	5	-10.559 (58) 0
17	17	O	7	1.196264 (16)	1	122.533 (38)	2	102.052 (59) 0
18	18	O	7	1.322560 (17)	1	-111.245 (39)	2	-77.254 (60) 0
19	19	C	18	1.440833 (18)	7	115.907 (40)	1	-179.604 (61) 0
20	20	H	19	0.934096 (19)	18	110.296 (41)	7	178.879 (62) 0
21	21	H	19	0.792386 (20)	18	109.029 (42)	7	-47.307 (63) 0
22	22	H	19	0.928466 (21)	18	110.944 (43)	7	50.900 (64) 0
23	23	H	3	0.887293 (22)	4	119.957 (44)	5	176.795 (65) 0
24	24	H	5	0.901565 (23)	4	121.567 (45)	3	-178.313 (66) 0

STOICHIOMETRY CBH5N3O8

SCF DONE: E(RHF) = -1062.92339579

EIGENVALUES — -0.37469 -0.32483 -0.32381 -0.32239 0.10480

Estimated ionization potential: 8.78 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.975266	0.025
2	C	5.880043	0.120
3	C	6.086838	-0.087
4	C	5.872820	0.127
5	C	6.076690	-0.077
6	C	5.886064	0.114
7	C	5.615164	0.385
8	N	6.818939	0.181
9	N	6.818394	0.182
10	N	6.817896	0.182
11	O	8.195753	-0.196
12	O	8.181190	-0.181
13	O	8.188783	-0.189
14	O	8.190735	-0.191
15	O	8.197226	-0.197
16	O	8.183581	-0.184
17	O	8.260313	-0.260
18	C	8.240812	-0.241
19	C	6.278682	-0.279
20	F	0.852278	0.148
21	F	0.840594	0.159
22	H	0.848691	0.151
23	H	0.847549	0.152
24	H	0.845699	0.154

DIPOLE MOMENT (DEBYE): X=-0.7273 Y=-0.9971 Z=-0.3363 TOTAL= 1.2792

V-mid: C2-N8: 0.216

C4-N9: 0.223

C6-N10: 0.213

Bond Order: C2-N8: 1.23

C4-N9: 1.24

C6-N10: 1.24

N8-O11: 1.95

N8-O12: 2.03

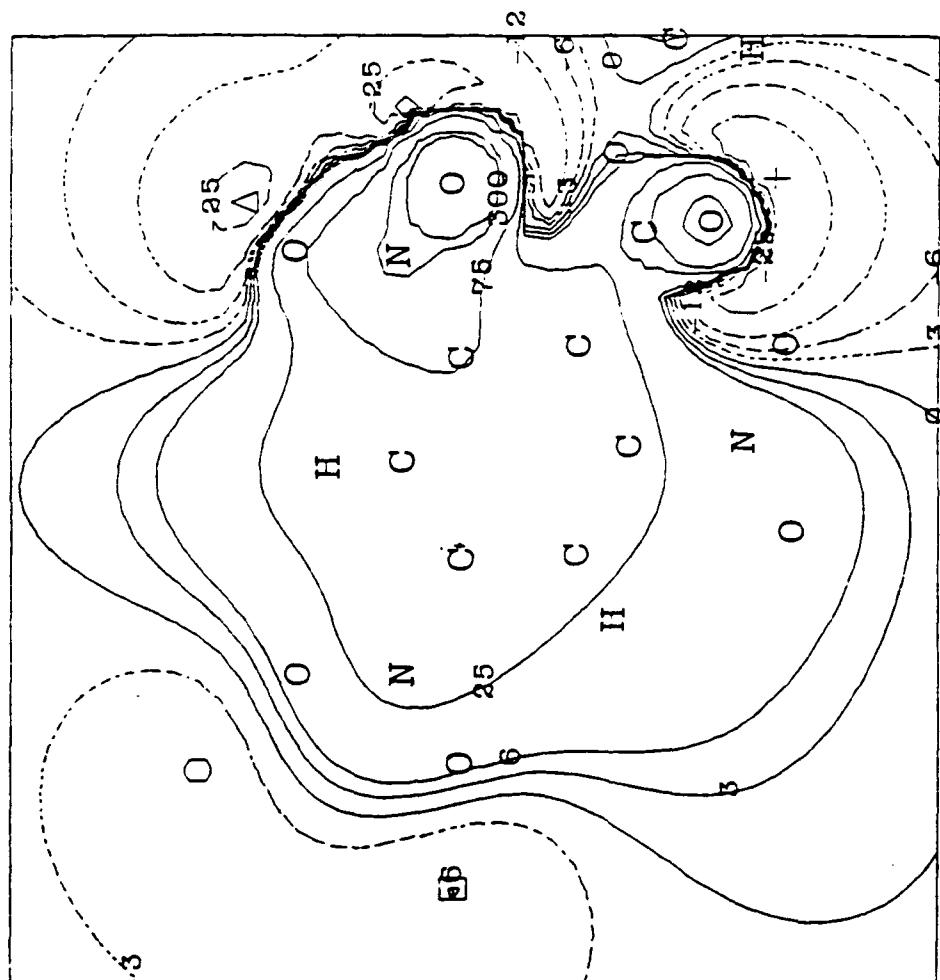
N9-O13: 2.02

N9-O14: 1.98

N10-O15: 1.96

N10-O16: 2.02

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0



MINIMA	
□	-6.024
○	-5.227
△	-30.139
†	-42.093
◇	-36.414

Figure N-1. Calculated electrostatic potential, in kcal/mole, of methyl-2,4,6-trinitrobenzoate, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0

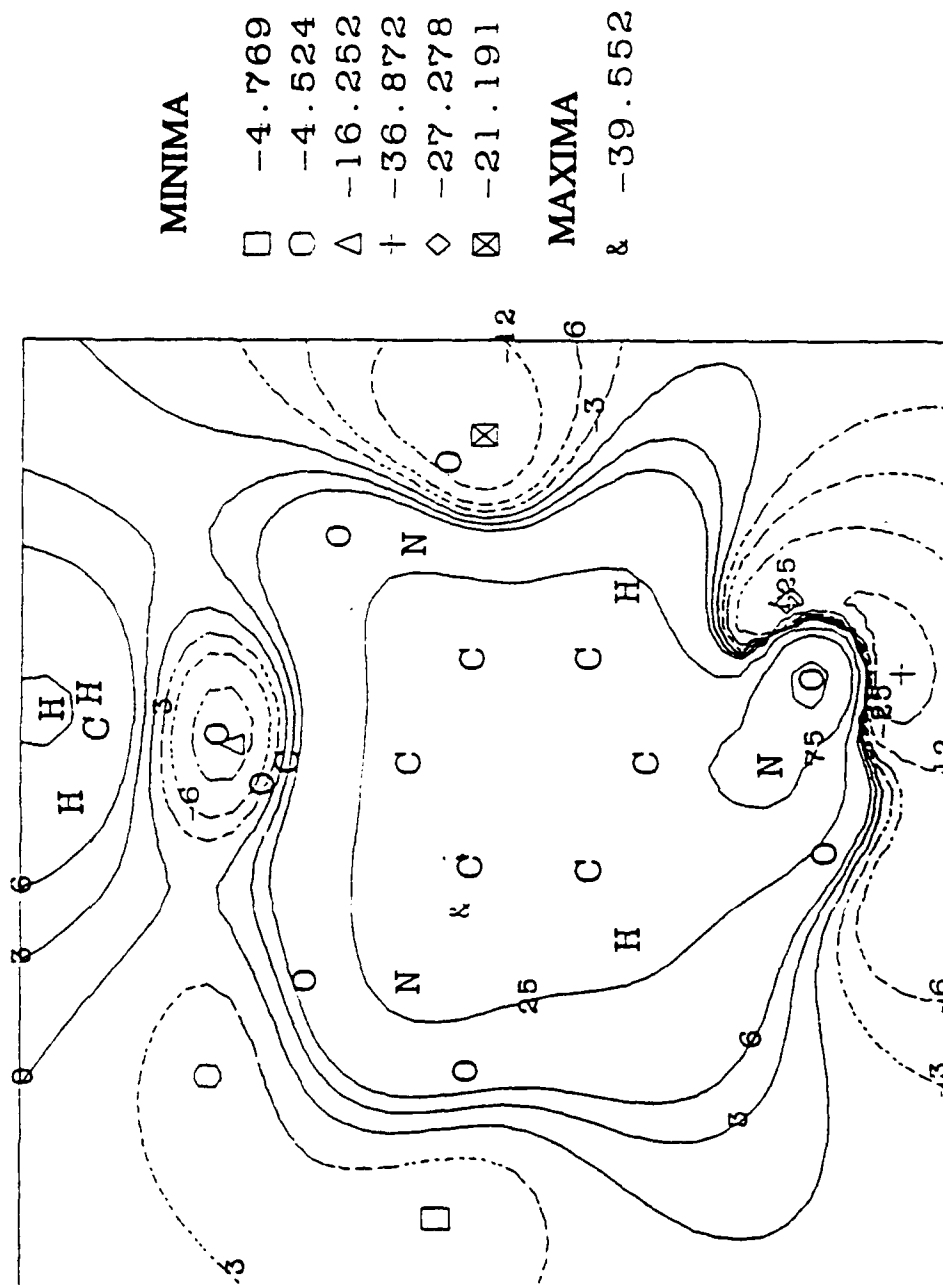
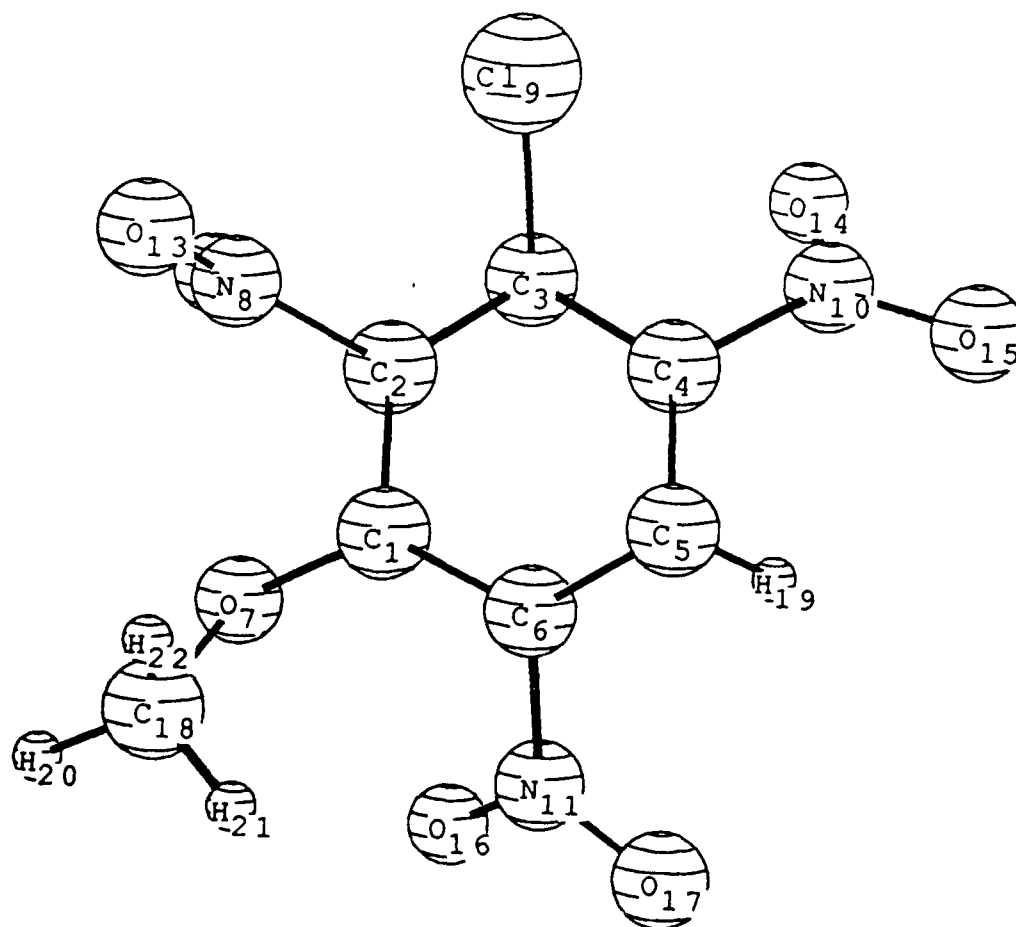


Figure N-2. Calculated electrostatic potential, in kcal/mole, of methyl-2,4,6-trinitrobenzoate, in the plane 1.75 Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX O
3-CHLORO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens are H19-O15 (2.40 Å), and H21-O16 (2.49 Å).

The N10 and N11 nitro groups are both rotated out of the mean plane of the benzene ring by about 34°, while the N8 nitro groups is essentially perpendicular to the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.393000(1)				
3	3	C	2	1.379882(2)	1	124.169(22)		
4	4	C	3	1.397787(3)	2	117.131(23)	1	-1.982(42)
5	5	C	4	1.375273(4)	3	120.917(24)	2	-1.185(43)
6	6	C	5	1.379063(5)	4	119.743(25)	3	3.635(44)
7	7	O	1	1.337936(6)	2	117.416(26)	3	-175.920(45)
8	8	N	2	1.475404(7)	3	119.302(27)	4	176.836(46)
9	9	Cl	3	1.708597(8)	4	123.881(28)	5	176.182(47)
10	10	N	4	1.467148(9)	5	116.929(29)	6	-175.679(48)
11	11	N	6	1.470114(10)	5	116.868(30)	4	175.101(49)
12	12	O	8	1.206072(11)	2	116.279(31)	1	-93.668(50)
13	13	O	8	1.209100(12)	2	117.012(32)	1	87.023(51)
14	14	O	10	1.210823(13)	4	117.965(33)	5	145.702(52)
15	15	O	10	1.217797(14)	4	116.529(34)	5	-33.103(53)
16	16	O	11	1.213555(15)	6	117.798(35)	5	-143.428(54)
17	17	O	11	1.213311(16)	6	117.378(36)	5	34.636(55)
18	18	C	7	1.436348(17)	1	117.841(37)	2	-116.169(56)
19	19	H	5	0.954598(18)	4	115.499(38)	3	176.687(57)
20	20	H	18	0.973907(19)	7	110.200(39)	1	179.977(58)
21	21	H	18	0.963601(20)	7	110.585(40)	1	-60.623(59)
22	22	H	18	0.961951(21)	7	110.815(41)	1	60.344(60)

STOICHIOMETRY C7H4ClN3O7

SCF DONE: E(RHF) = -1408.06215783

Alpha eigenvalues — -0.35582 -0.32435 -0.32228 -0.32083 0.10979

Estimated ionization potential: 8.73 ev

Total atomic charges:

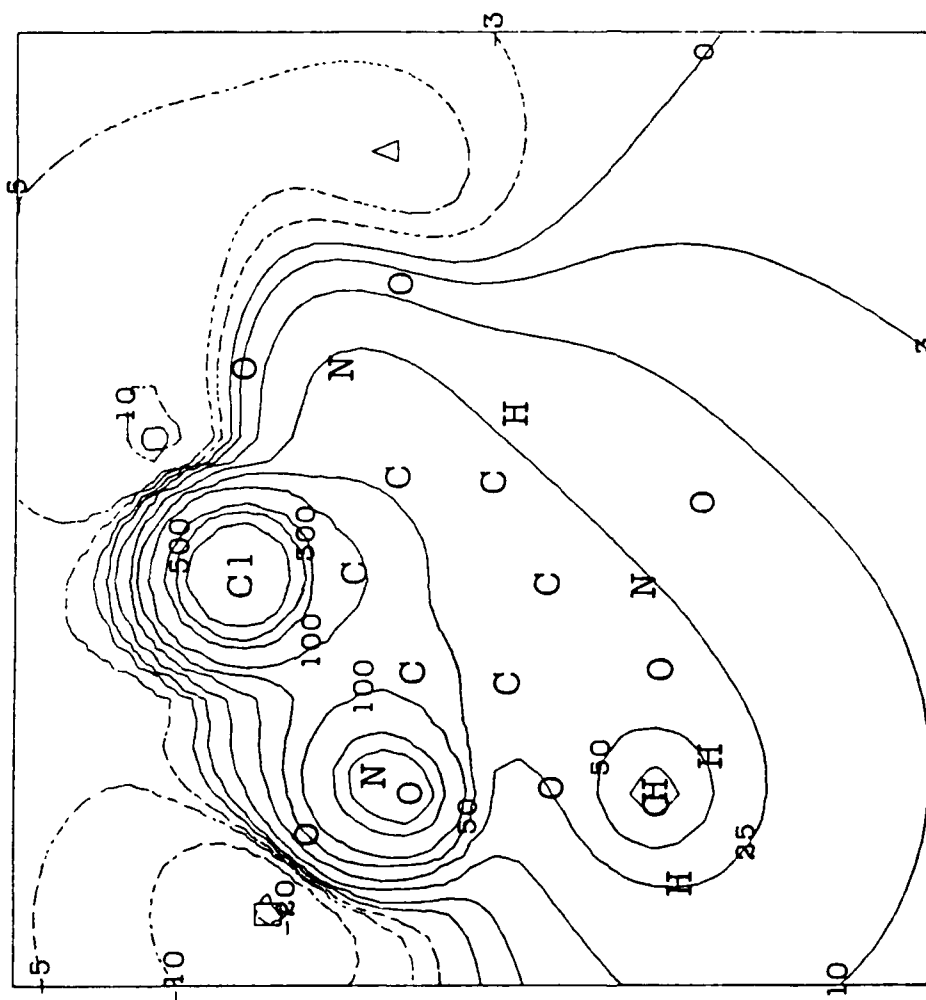
1
 1 C 0.192606
 2 C 0.089377
 3 C 0.057532
 4 C 0.101570
 5 C -0.053390
 6 C 0.080864
 7 O -0.231147
 8 N 0.190374
 9 Cl -0.028886
 10 N 0.178105
 11 N 0.175684
 12 O -0.173706
 13 O -0.189534
 14 O -0.176087
 15 O -0.192282
 16 O -0.187936
 17 O -0.189789
 18 C -0.165813
 19 H 0.147707
 20 H 0.136505
 21 H 0.118657
 22 H 0.119587

Dipole moment (Debye):

X= -2.1747 Y= -0.2494 Z= 1.2918 Tot= 2.5418

Bond Order: C2-N8: 1.23	V-mid: C2-N8: 0.201
C4-N10: 1.25	C4-N10: 0.202
C6-N11: 1.24	C6-N11: 0.185
N8-O12: 2.01	
N8-O13: 2.00	
N10-O14: 1.98	
N10-O15: 1.95	
N11-O16: 1.97	
N11-O17: 1.97	

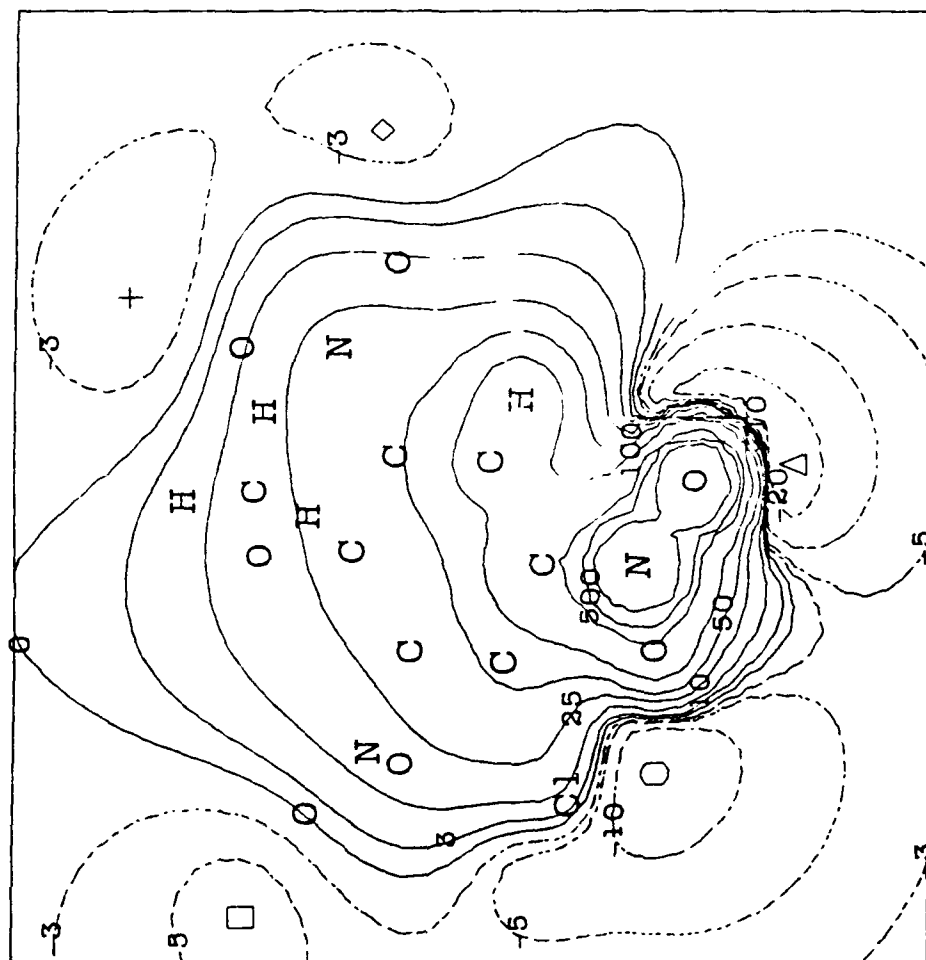
-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA
□ -20.7
○ -10.8
△ -6.6

Figure O-1. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA

□ -5.8
○ -16.6
△ -28.7
+ -4.9
◇ -3.8

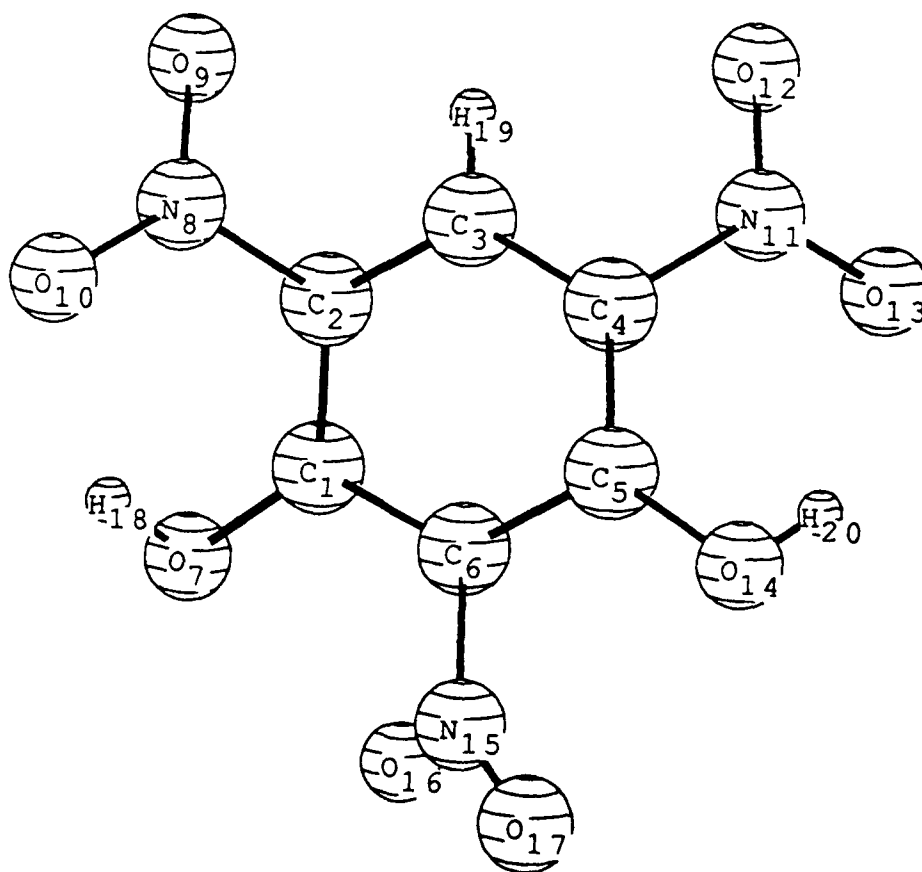
Figure O-2. Calculated electrostatic potential, in kcal/mole, of 3-chloro-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX P

STYPHNIC ACID

The short distances between non-bonded hydrogens and oxygens are H19-O12 (2.40 Å), H20-O13 (1.91 Å), H9-O9 (2.40 Å), and H18-O10 (1.91 Å).

The N8 and N11 nitro groups are essentially co-planar with the mean plane of the benzene ring, while the N15 nitro group is rotated by about 66°.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA J
1	1	C						
2	2	C	1	1.402080 (1)				
3	3	C	2	1.369661 (2)	1	121.310 (20)		
4	4	C	3	1.369663 (3)	2	120.570 (21)	1	-1.095 (38) 0
5	5	C	4	1.402073 (4)	3	121.310 (22)	2	-1.094 (39) 0
6	6	C	5	1.392829 (5)	4	116.460 (23)	3	2.086 (40) 0
7	7	O	1	1.326033 (6)	6	116.970 (24)	5	179.558 (41) 0
8	8	N	2	1.455679 (7)	3	118.669 (25)	4	177.595 (42) 0
9	9	O	8	1.216943 (8)	2	118.685 (26)	3	2.789 (43) 0
10	10	O	8	1.235027 (9)	2	118.272 (27)	3	-176.579 (44) 0
11	11	N	4	1.455678 (10)	5	120.009 (28)	6	-176.587 (45) 0
12	12	O	11	1.216944 (11)	4	118.685 (29)	5	-178.504 (46) 0
13	13	O	11	1.235036 (12)	4	118.273 (30)	5	2.129 (47) 0
14	14	O	5	1.326028 (13)	6	116.969 (31)	1	179.558 (48) 0
15	15	N	6	1.467534 (14)	1	118.079 (32)	2	178.989 (49) 0
16	16	O	15	1.217419 (15)	6	117.777 (33)	1	66.121 (50) 0
17	17	O	15	1.217422 (16)	6	117.776 (34)	1	-113.879 (51) 0
18	18	H	7	0.838803 (17)	1	110.127 (35)	2	-14.286 (52) 0
19	19	H	3	0.895145 (18)	4	119.715 (36)	5	178.906 (53) 0
20	20	H	14	0.838806 (19)	5	110.128 (37)	6	165.079 (54) 0

STOICHIOMETRY: C6H3N3O8

E= -986.441730465

EIGENVALUES — -0.33180 -0.29774 0.11913 0 11944 0.18924

Estimated ionization potential: 8.10 ev

TOTAL ATOMIC CHARGES.

	1	Net Charges
1 C	5.784320	+0.22
2 C	5.951153	+0.05
3 C	6.060130	-0.06
4 C	5.951145	+0.05
5 C	5.784320	+0.22
6 C	5.947836	+0.05
7 O	8.352258	-0.35
8 N	6.829713	+0.17
9 O	8.169836	-0.17
10 O	8.228012	-0.23
11 N	6.829721	+0.17
12 O	8.169836	-0.17
13 O	8.228023	-0.23
14 O	8.352260	-0.35
15 N	6.816398	+0.18
16 O	8.186697	-0.19
17 O	8.186698	-0.19
18 H	0.663593	+0.34
19 H	0.844464	+0.16
20 H	0.663588	+0.34

DIPOLE MOMENT (DEBYE): X=-0.0496 Y= 0.0296 Z= 1.7812 TOTAL= 1.7821

V_{mid}: C₂-N₈: 0.159
 C₄-N₁₁: 0.159
 C₆-N₁₅: 0.170

Bond Orders: C₂-N₈: 1.28
 C₄-N₁₁: 1.28
 C₆-N₁₅: 1.25
 N₈-O₉: 2.11
 N₈-O₁₀: 2.02
 N₁₁-O₁₂: 2.11
 N₁₁-O₁₃: 2.02
 N₁₅-O₁₆: 2.11
 N₁₅-O₁₇: 2.11

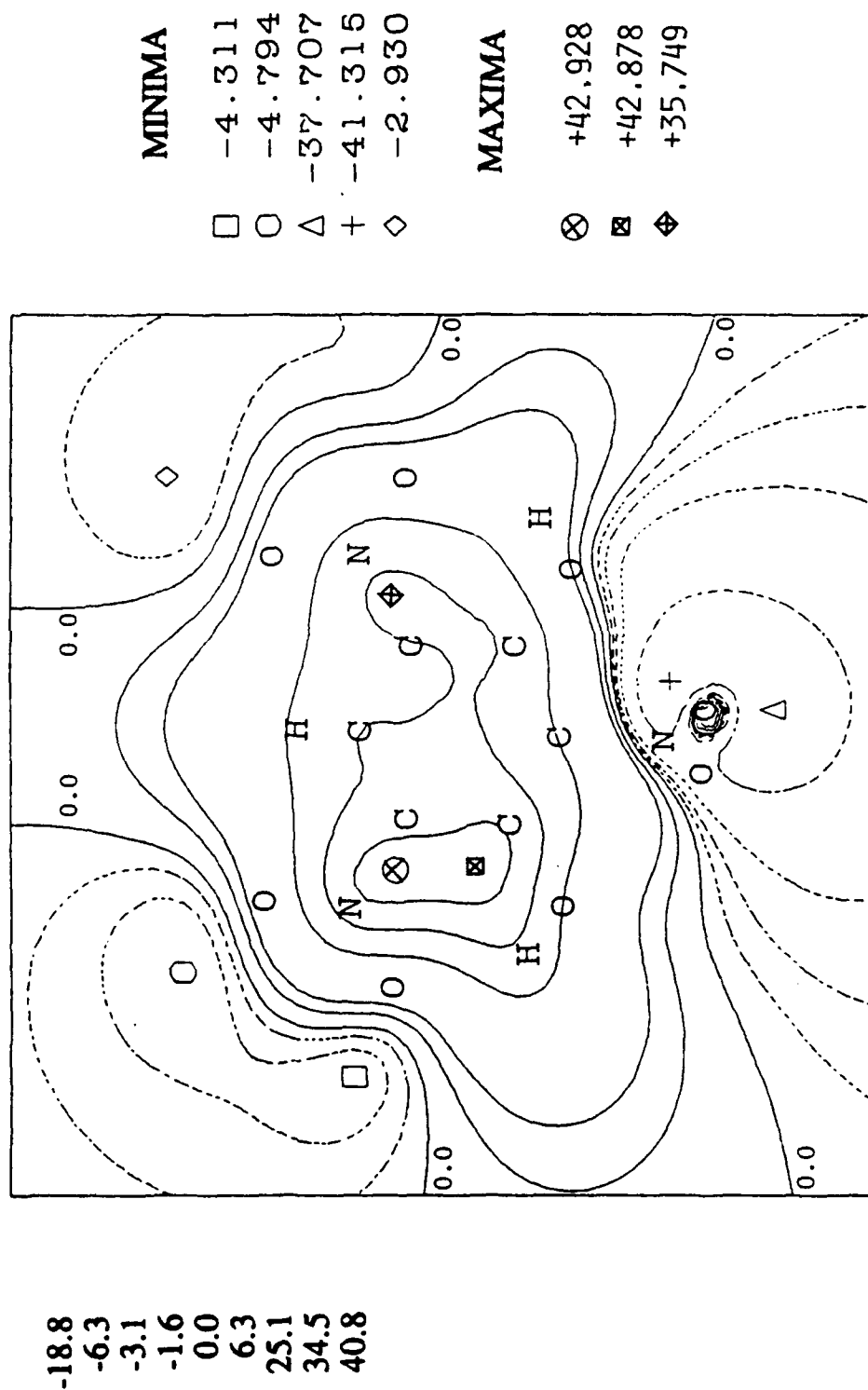


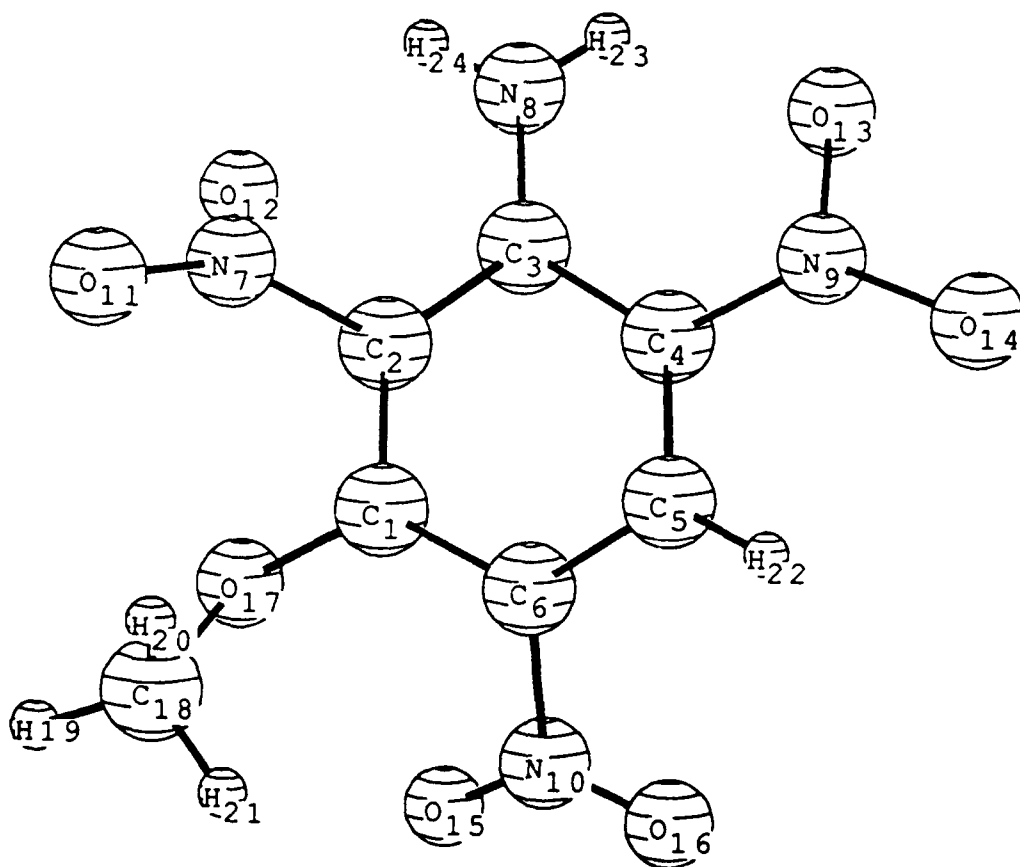
Figure P-1. Calculated electrostatic potential, in kcal/mole, of styphnic acid, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Q

3-AMINO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H24-O12 (2.15 Å), H23-O13 (2.01 Å), H22-O14 (2.35 Å) and H21-O15 (2.37 Å).

The N7 is rotated out of the mean plane of the benzene ring by more than 50°, and the N9 and N10 nitro groups are rotated by approximately 10° and 20°, respectively. The amine group (N8) is almost planar with respect to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J

1	1	C							
2	2	C	1	1.390000 (1)					
3	3	C	2	1.410000 (2)	1	125.700 (24)			
4	4	C	3	1.430000 (3)	2	113.400 (25)	1	-7.800 (46)	0
5	5	C	4	1.380000 (4)	3	122.100 (26)	2	6.750 (47)	0
6	6	C	5	1.380000 (5)	4	121.000 (27)	3	-1.300 (48)	0
7	7	N	2	1.460000 (6)	3	117.300 (28)	4	170.800 (49)	0
8	8	N	3	1.320000 (7)	4	123.600 (29)	5	-177.200 (50)	0
9	9	N	4	1.460000 (8)	5	115.800 (30)	6	179.300 (51)	0
10	10	N	6	1.460000 (9)	5	116.800 (31)	4	173.000 (52)	0
11	11	O	7	1.210000 (10)	2	119.200 (32)	3	-127.100 (53)	0
12	12	O	7	1.240000 (11)	2	116.800 (33)	3	51.100 (54)	0
13	13	O	9	1.230000 (12)	4	118.700 (34)	5	171.400 (55)	0
14	14	O	9	1.210000 (13)	4	119.100 (35)	5	-9.800 (56)	0
15	15	O	10	1.200000 (14)	6	119.100 (36)	5	-158.400 (57)	0
16	16	O	10	1.210000 (15)	6	118.100 (37)	5	17.990 (58)	0
17	17	O	1	1.330000 (16)	2	118.100 (38)	3	-173.700 (59)	0
18	18	C	17	1.430000 (17)	1	117.500 (39)	2	-113.800 (60)	0
19	19	H	18	0.950000 (18)	17	106.100 (40)	1	173.050 (61)	0
20	20	H	18	0.960000 (19)	17	112.000 (41)	1	53.300 (62)	0
21	21	H	18	0.960000 (20)	17	109.500 (42)	1	-68.850 (63)	0
22	22	H	5	0.930000 (21)	4	119.100 (43)	3	171.600 (64)	0
23	23	H	8	0.850000 (22)	3	118.810 (44)	2	-177.700 (65)	0
24	24	H	8	0.870000 (23)	3	117.380 (45)	2	3.240 (66)	0

STOICHIOMETRY C7H6N4O7

E(RHF)= -1005.60972021 A.U.

EIGENVALUES -- -0.30696 0.12681 0.14417 0.18365 0.23639

Estimated ionization potential: 8.36 ev

TOTAL ATOMIC CHARGES.			
		1	Net Charge
1	C	5.792603	0.217
2	C	5.961544	0.038
3	C	5.778044	0.222
4	C	5.945189	0.055
5	C	6.050720	-0.051
6	C	5.952368	0.048
7	N	6.833561	0.166
8	N	7.554206	-0.554
9	N	6.827607	0.172
10	N	6.819568	0.180
11	O	8.181589	-0.182
12	O	8.212943	-0.213
13	O	8.225226	-0.225
14	O	8.186964	-0.187
15	O	8.202570	-0.203
16	O	8.208008	-0.208
17	O	8.234741	-0.235
18	C	6.171876	-0.172
19	H	0.862767	0.137
20	H	0.878724	0.121
21	H	0.876168	0.124
22	H	0.849407	0.151
23	H	0.686439	0.324
24	H	0.707169	0.293

DIPOLE MOMENT (DEBYE): X=-1.1358 Y=-1.3317 Z= 1.3143 TOTAL= 2.1888

V-mid: N7-C2: 0.148
 N9-C4: 0.165
 N10-C6: 0.165

BOND ORDER: N7-C2: 1.27
 N9-C4: 1.27
 N10-C6: 1.27
 O11-N7: 1.99
 O12-N7: 1.85
 O13-N9: 1.89
 O14-N9: 1.99
 O15-N10: 2.04
 O16-N11: 1.99

-25.100
 -12.550
 -6.275
 -3.138
 0.000
 3.138
 6.275
 25.100
 50.201
 62.751
 313.754
 627.509
 0.000

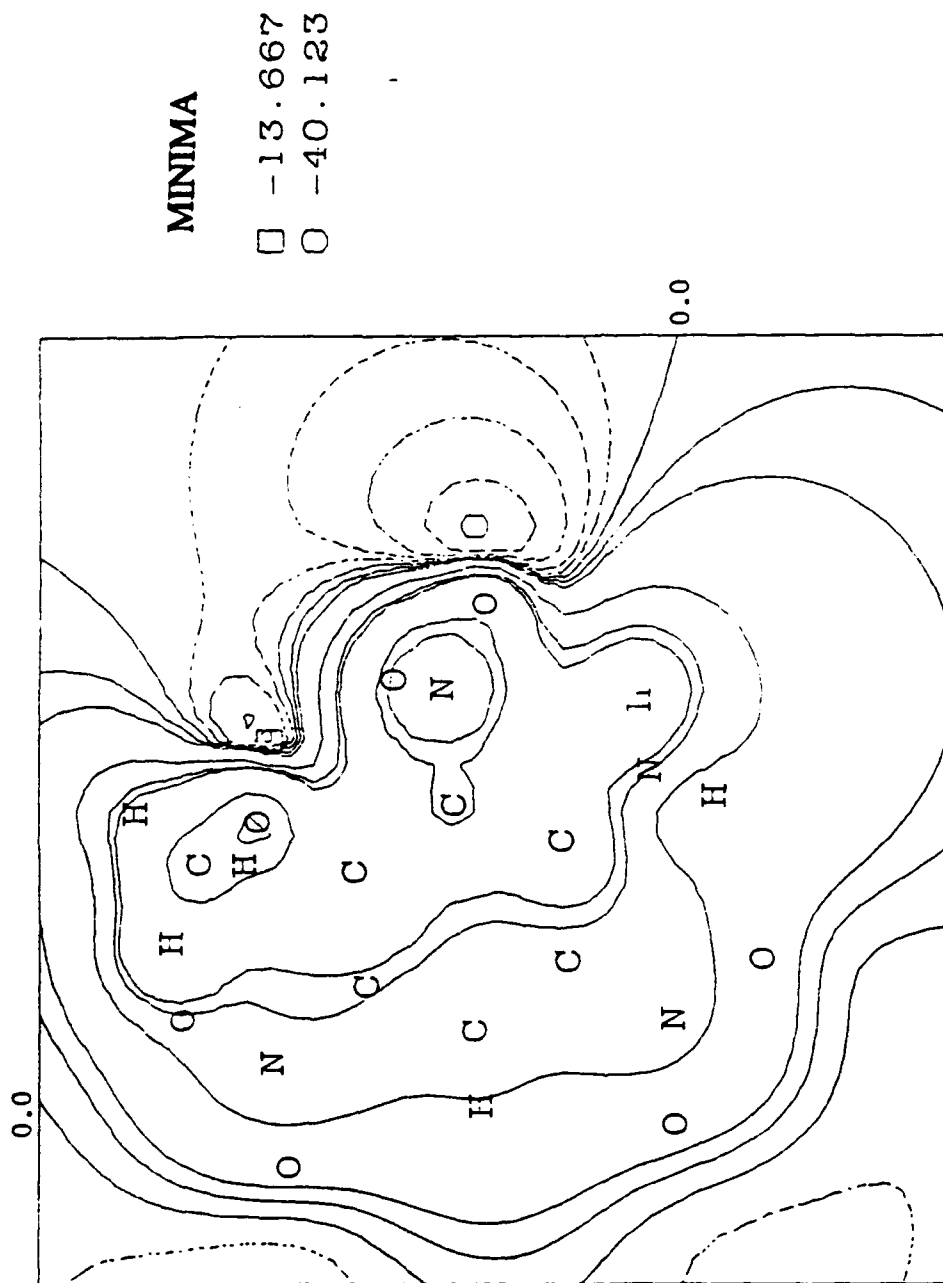


Figure Q-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroanisole, in the plane 1.75 Å above the N10 nitro group located in the upper left corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.100
 -12.550
 -6.275
 -3.138
 0.000
 3.138
 6.275
 25.100
 50.201
 62.751
 313.754
 627.509
 0.000

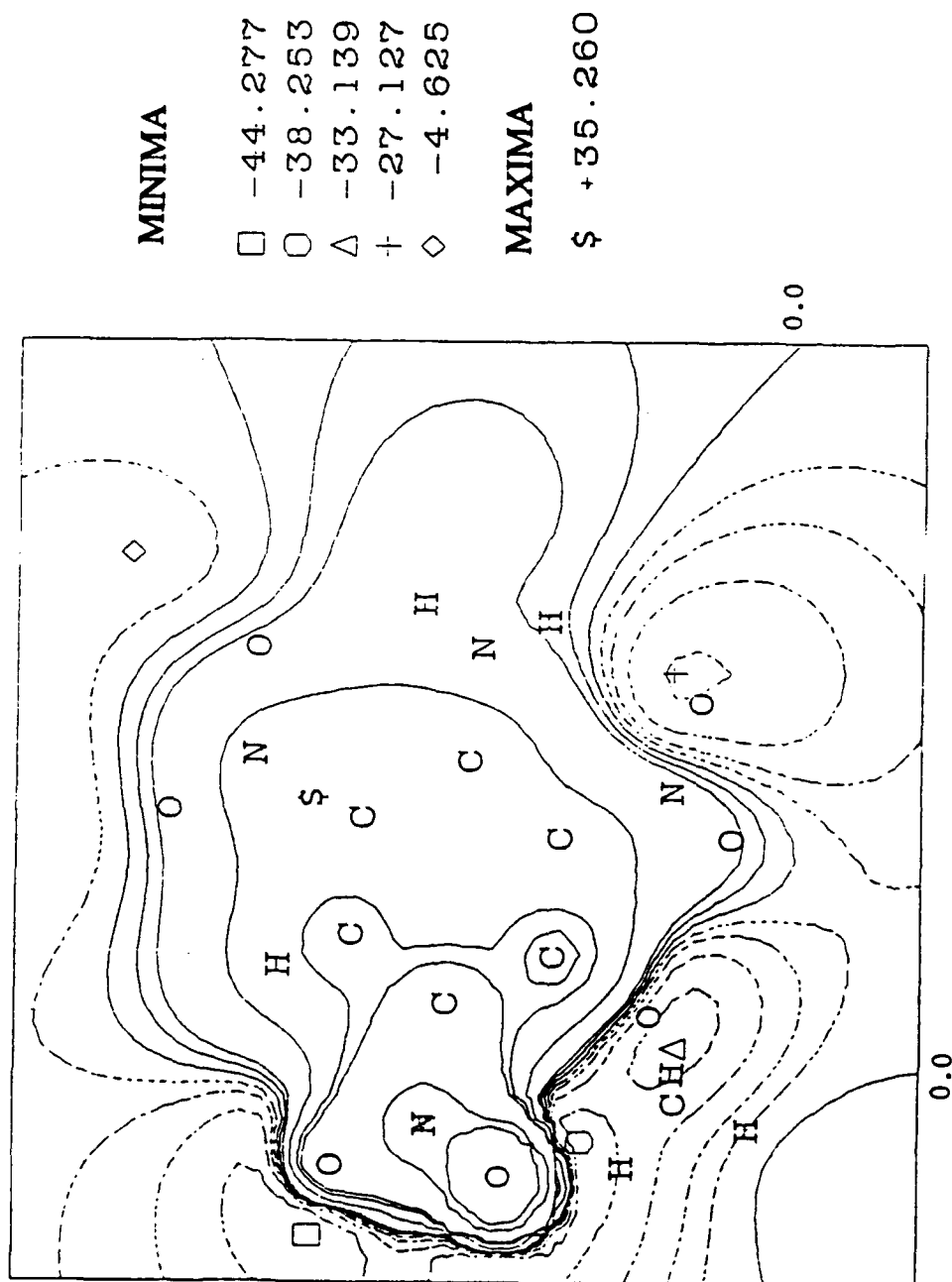
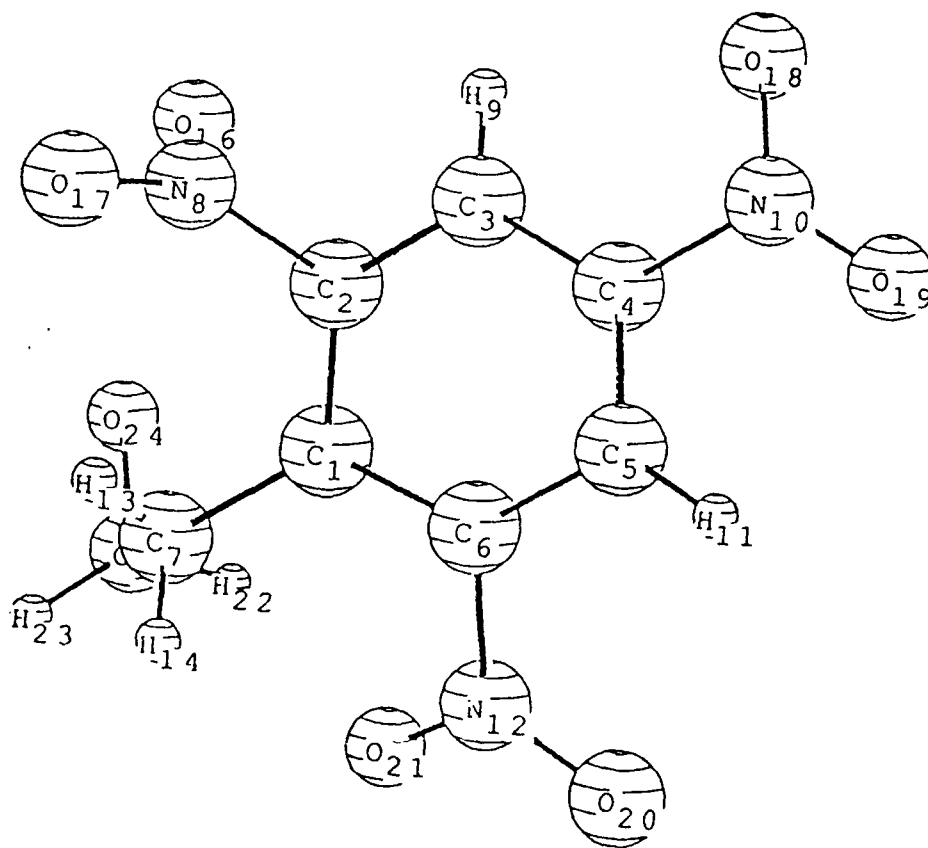


Figure Q-2. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroanisole, in the plane 1.75 Å above the N9 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX R
2,4,6-TRINITROPHENYLETHANOL

The short distances between non-bonded hydrogens and oxygens are H9-O18 (2.36 Å), H11-O19 (2.51 Å) and H11-O20 (2.40 Å).

The N10 nitro group is essentially planar, while the N8 and N12 nitro groups are rotated by about 53° and 38°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.405790 (1)					
3	3	C	2	1.385454 (2)	1	124.441 (25)			
4	4	C	3	1.375723 (3)	2	117.275 (26)	1	-3.639 (48)	0
5	5	C	4	1.375494 (4)	3	122.596 (27)	2	1.748 (49)	0
6	6	C	5	1.387018 (5)	4	117.247 (28)	3	1.633 (50)	0
7	7	C	1	1.511773 (6)	2	122.283 (29)	3	-177.102 (51)	0
8	8	N	2	1.473278 (7)	3	114.345 (30)	4	176.070 (52)	0
9	9	H	3	0.935064 (8)	4	118.949 (31)	5	-179.191 (53)	0
10	10	N	4	1.474252 (9)	5	119.211 (32)	6	-178.828 (54)	0
11	11	H	5	0.969896 (10)	6	117.339 (33)	1	177.776 (55)	0
12	12	N	6	1.479221 (11)	1	120.688 (34)	2	-179.154 (56)	0
13	13	H	7	0.892075 (12)	1	107.604 (35)	2	-35.424 (57)	0
14	14	H	7	1.020122 (13)	1	116.186 (36)	2	-144.012 (58)	0
15	15	C	7	1.516479 (14)	1	111.660 (37)	2	86.695 (59)	0
16	16	O	8	1.226461 (15)	2	117.448 (38)	3	52.840 (60)	0
17	17	O	8	1.214653 (16)	2	118.009 (39)	3	-123.320 (61)	0
18	18	O	10	1.221396 (17)	4	117.365 (40)	5	178.357 (62)	0
19	19	O	10	1.226018 (18)	4	117.880 (41)	5	-1.925 (63)	0
20	20	O	12	1.222992 (19)	6	116.957 (42)	1	-142.921 (64)	0
21	21	O	12	1.223812 (20)	6	118.327 (43)	1	38.341 (65)	0
22	22	H	15	1.113303 (21)	7	111.293 (44)	1	49.750 (66)	0
23	23	H	15	1.101230 (22)	7	105.243 (45)	1	176.128 (67)	0
24	24	O	15	1.437708 (23)	7	108.002 (46)	1	-66.161 (68)	0
25	25	H	24	0.667343 (24)	15	116.108 (47)	7	173.061 (69)	0

STOICHIOMETRY C8H7N3O7

SCF DONE: E(RHF) = -989.592181678

EIGENVALUES — -0.30175 0.12168 0.13401 0.18800 0.22444

Estimated ionization potential: 8.22 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.933057	0.067
2	C	5.886905	0.114
3	C	6.070620	-0.071
4	C	5.892277	0.108
5	C	6.060411	-0.060
6	C	5.903170	0.097
7	C	6.206240	-0.206
8	N	6.821298	0.178
9	H	0.854565	0.145
10	N	6.830005	0.170
11	H	0.856326	0.144
12	N	6.832640	0.167
13	H	0.860920	0.139
14	H	0.884685	0.115
15	C	5.943004	0.057
16	O	8.186415	-0.186
17	O	8.193307	-0.193
18	O	8.191157	-0.191
19	O	8.190719	-0.191
20	O	8.159051	-0.189
21	O	8.197190	-0.197
22	H	0.826404	0.074
23	H	0.927182	0.075
24	O	8.530079	-0.530
25	H	0.632393	0.368

DIPOLE MOMENT (DEBYE): X=-1.2233 Y= 1.1284 Z=-2.0872 TOTAL= 2.6695

V-mid: N8-C2: 0.210

N10-C4: 0.200

N12-C6: 0.189

Bond Order: N8-C2: 1.23

N10-C4: 1.23

N12-C6: 1.22

O16-N8: 1.91

O17-N8: 1.96

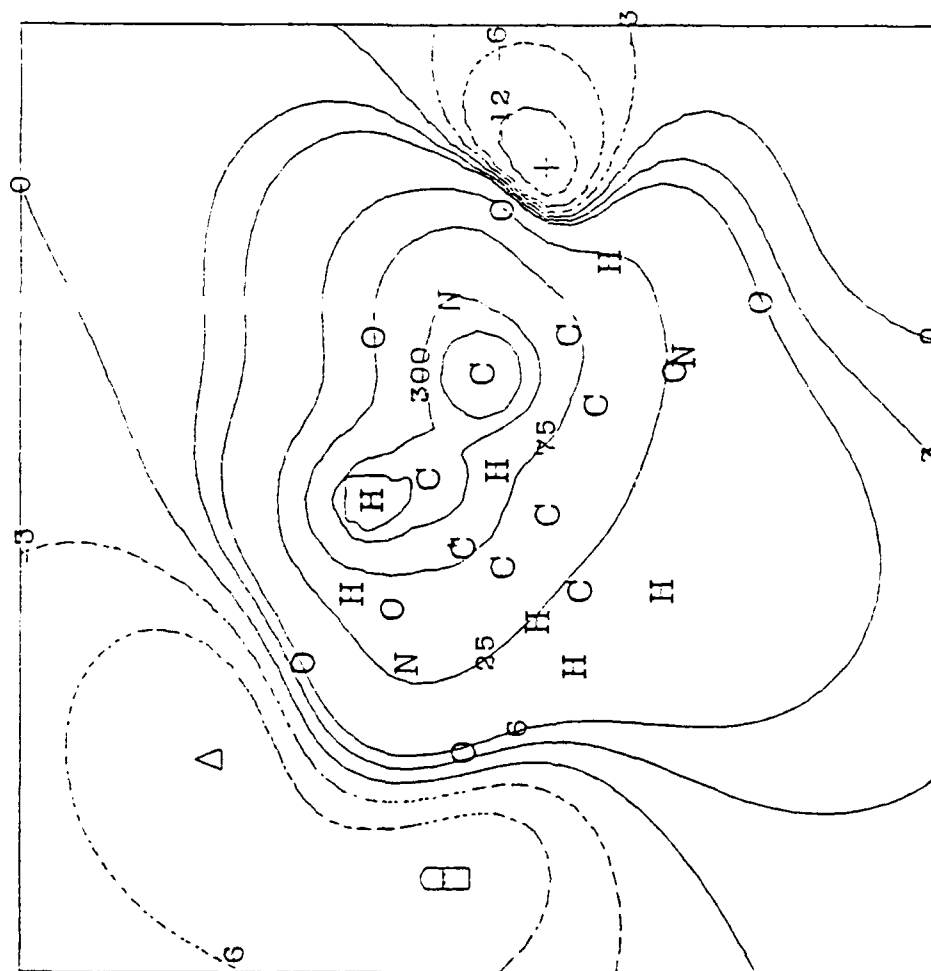
O18-N10: 1.93

O19-N10: 1.91

O20-N12: 1.92

O21-N12: 1.92

-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0

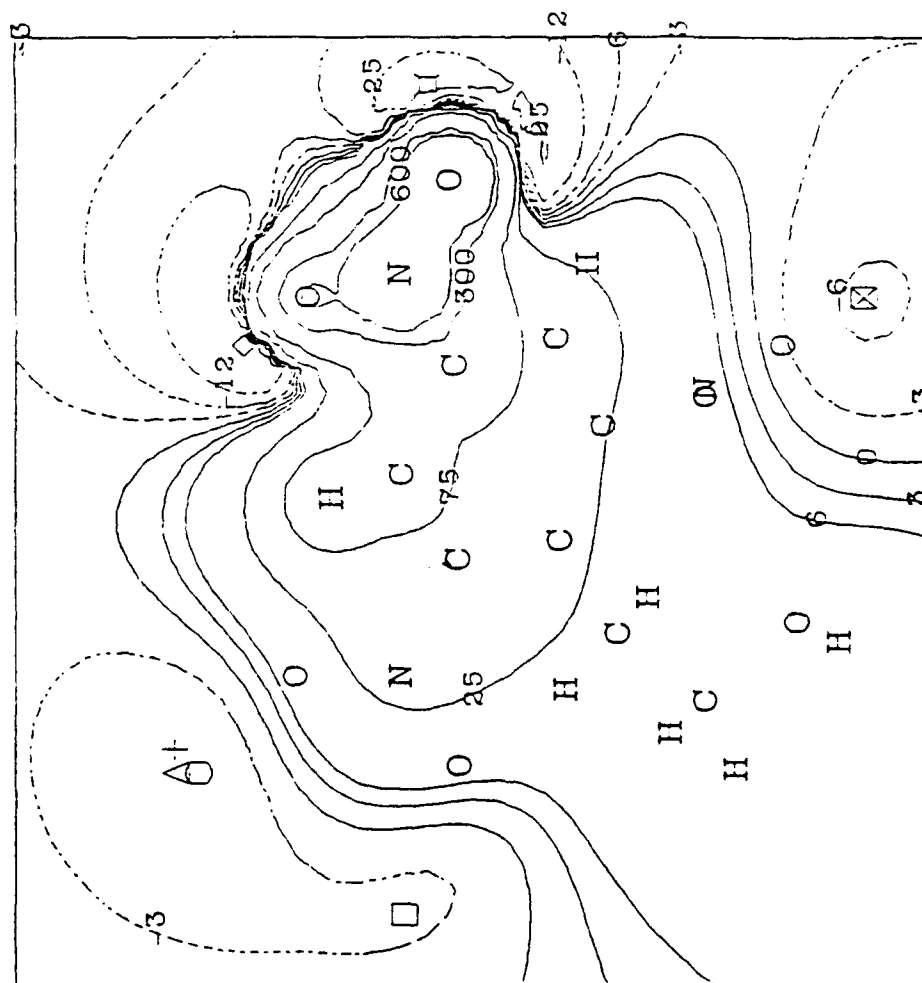


MINIMA

□ -8.603
○ -8.603
△ -9.099
+ -18.355

Figure R-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenylethanol, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0



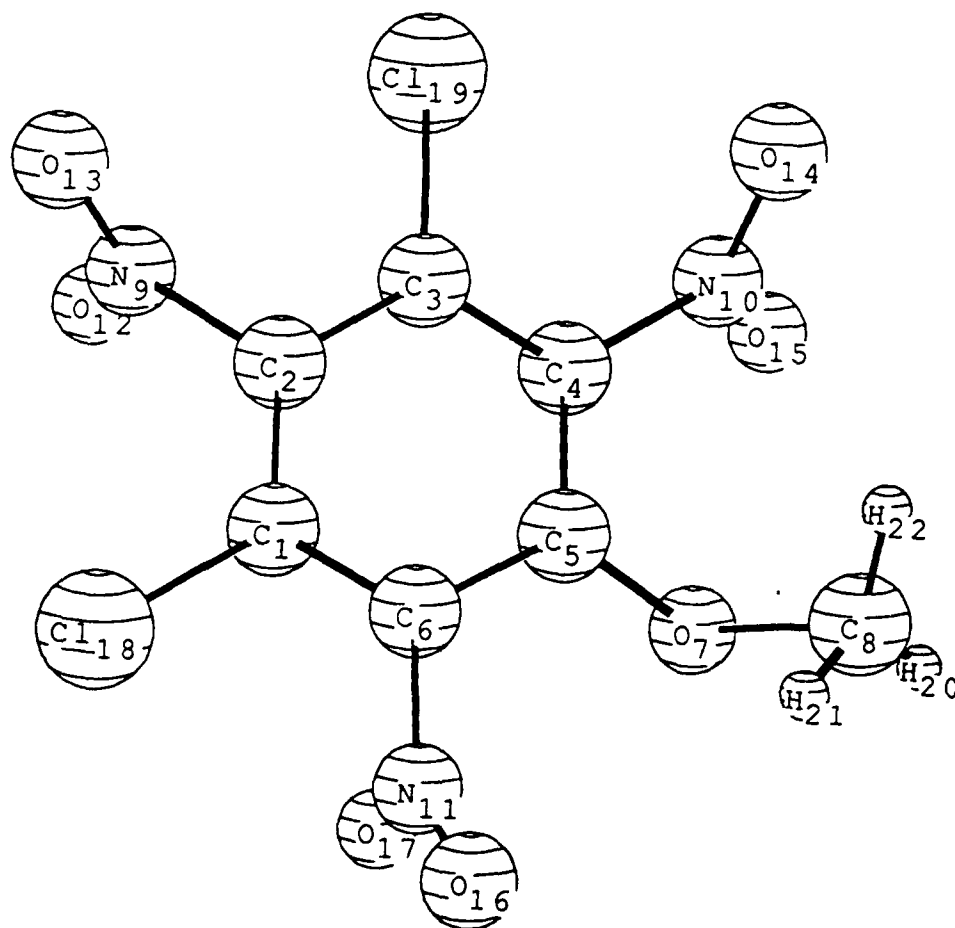
MINIMA

□ -3.401
○ -5.284
△ -5.284
+ -5.284
◇ -22.383
⊠ -6.350
⊞ -32.712

Figure R-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenylethanol, in the plane 1.75 Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX S
3,5-DICHLORO-2,4,6-TRINITROANISOLE

Nitro groups N9, N10 and N11 are rotated out of the plane by approximately 67°, 57° and 69°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J

1	1	C							
2	2	C	1	1.391000 (1)					
3	3	C	2	1.389206 (2)	1	121.473 (22)			
4	4	C	3	1.389143 (3)	2	118.999 (23)	1	1.346 (42)	0
5	5	C	4	1.395511 (4)	3	121.461 (24)	2	-1.551 (43)	0
6	6	C	5	1.395780 (5)	4	116.885 (25)	3	-0.898 (44)	0
7	7	O	5	1.340606 (6)	4	125.525 (26)	3	175.299 (45)	0
8	8	C	7	1.415489 (7)	5	121.652 (27)	4	56.587 (46)	0
9	9	N	2	1.476436 (8)	3	119.419 (28)	4	-177.119 (47)	0
10	10	N	4	1.474114 (9)	3	119.067 (29)	2	176.644 (48)	0
11	11	N	6	1.477912 (10)	5	115.855 (30)	4	-177.593 (49)	0
12	12	O	9	1.208747 (11)	2	117.506 (31)	1	-67.457 (50)	0
13	13	O	9	1.211470 (12)	2	117.410 (32)	1	111.862 (51)	0
14	14	O	10	1.212815 (13)	4	117.714 (33)	5	-122.340 (52)	0
15	15	O	10	1.221423 (14)	4	117.033 (34)	5	57.408 (53)	0
16	16	O	11	1.211646 (15)	6	117.282 (35)	5	68.605 (54)	0
17	17	O	11	1.218011 (16)	6	117.087 (36)	5	-111.539 (55)	0
18	18	Cl	1	1.710555 (17)	2	121.070 (37)	3	178.901 (56)	0
19	19	Cl	3	1.718514 (18)	4	120.773 (38)	5	-177.618 (57)	0
20	20	H	8	0.960422 (19)	7	115.442 (39)	5	-164.767 (58)	0
21	21	H	8	0.960380 (20)	7	93.642 (40)	5	81.700 (59)	0
22	22	H	8	0.959845 (21)	7	117.939 (41)	5	-32.636 (60)	0

STOICHIOMETRY C7H3CL2N3O7

SCF DONE: E(RHF) = -1865.25178442 A.U. AFTER 25 CYCLES

EIGENVALUES -- -0.33048 -0.32444 -0.32325 0.11187 0.12706

Estimated ionization potential: 8.81eV

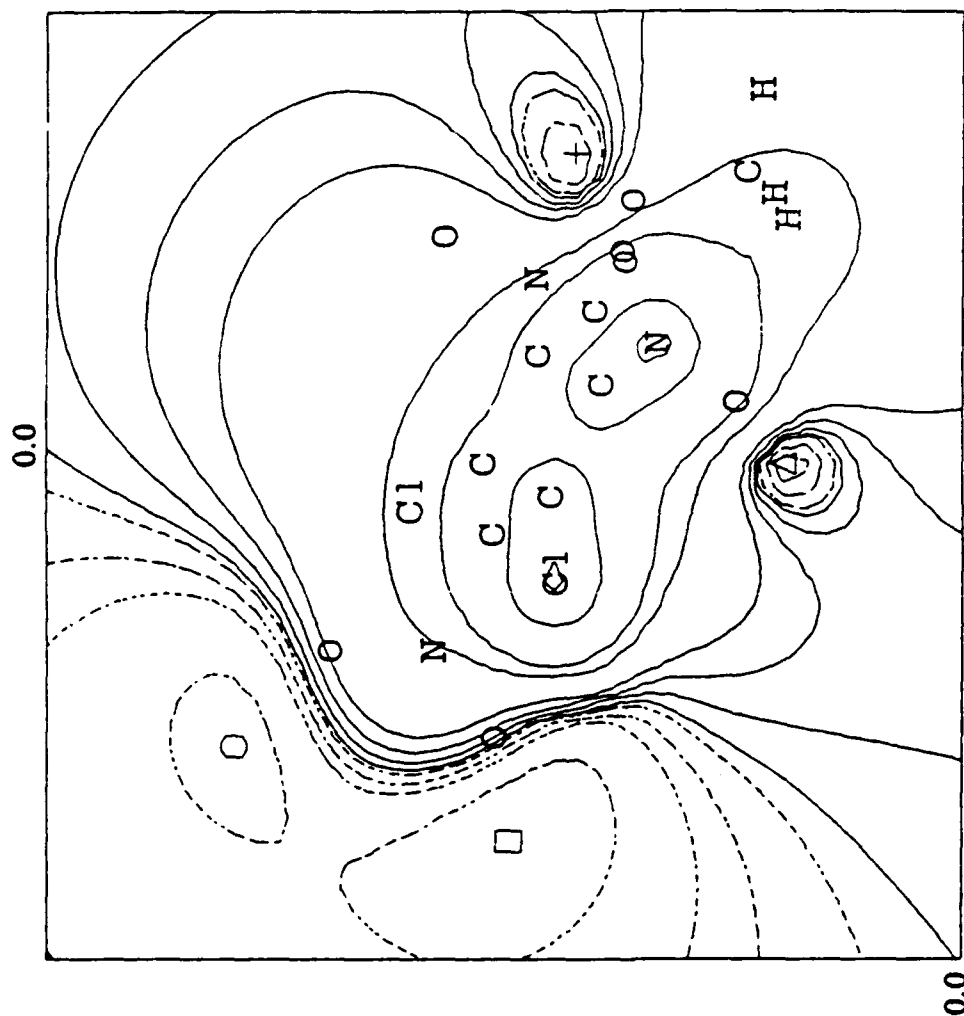
TOTAL ATOMIC CHARGES.		
	1	Net Charge
1	C	5.938767 0.061
2	C	5.901758 0.098
3	C	5.935152 0.065
4	C	5.924995 0.075
5	C	5.798703 0.201
6	C	5.914277 0.086
7	O	8.235248 -0.235
8	C	6.173128 -0.173
9	N	6.815860 0.184
10	N	6.826736 0.173
11	N	6.814434 0.186
12	O	8.174657 -0.175
13	O	8.176198 -0.176
14	O	8.175399 -0.175
15	O	8.179620 -0.180
16	O	8.184689 -0.185
17	O	8.173291 -0.173
18	Cl	17.024555 -0.025
19	Cl	17.029947 -0.030
20	H	0.858413 0.162
21	H	0.865099 0.135
22	H	0.879074 0.121

DIPOLE MOMENT (DEBYE): X= 2.5338 Y=-1.2750 Z=-0.5635 TOTAL= 2.8919

V-mid: N9-C2: 0.202
 N10-C4: 0.178
 N11-C6: 0.194

Bond Order: N9-C2: 1.22
 N10-C4: 1.23
 N11-C6: 1.22
 O12-N9: 1.99
 O13-N9: 1.98
 O14-N10: 1.97
 O15-N10: 1.93
 O16-N11: 1.98
 O17-N11: 1.95

0.000
-6.275
-3.138
-1.883
-0.628
1.255
3.138
6.275
31.375
62.751
313.754
627.509
0.000



MINIMA
□ -8.867
○ -7.135
△ -4.248
+ -2.999

Figure S-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75 Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

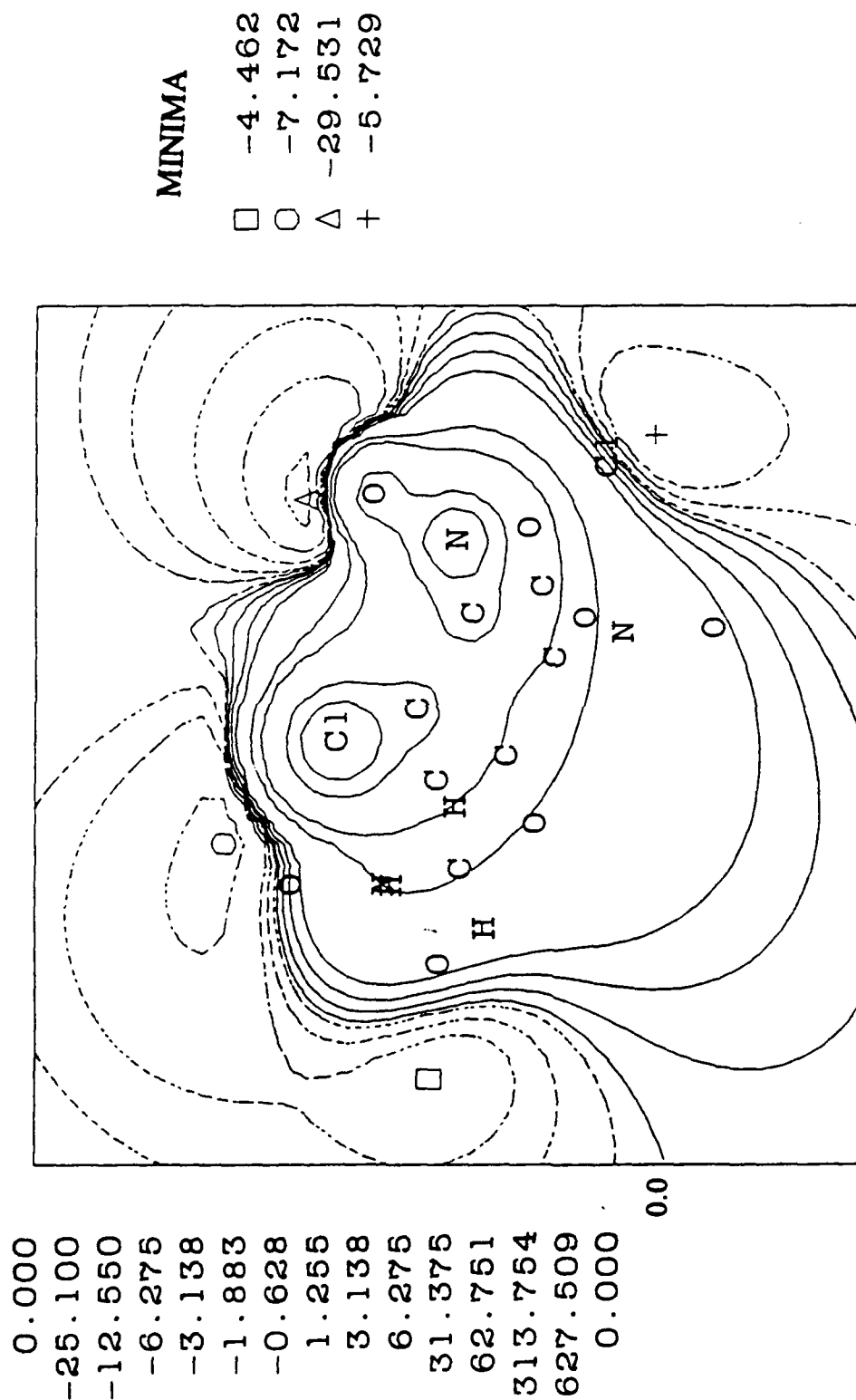
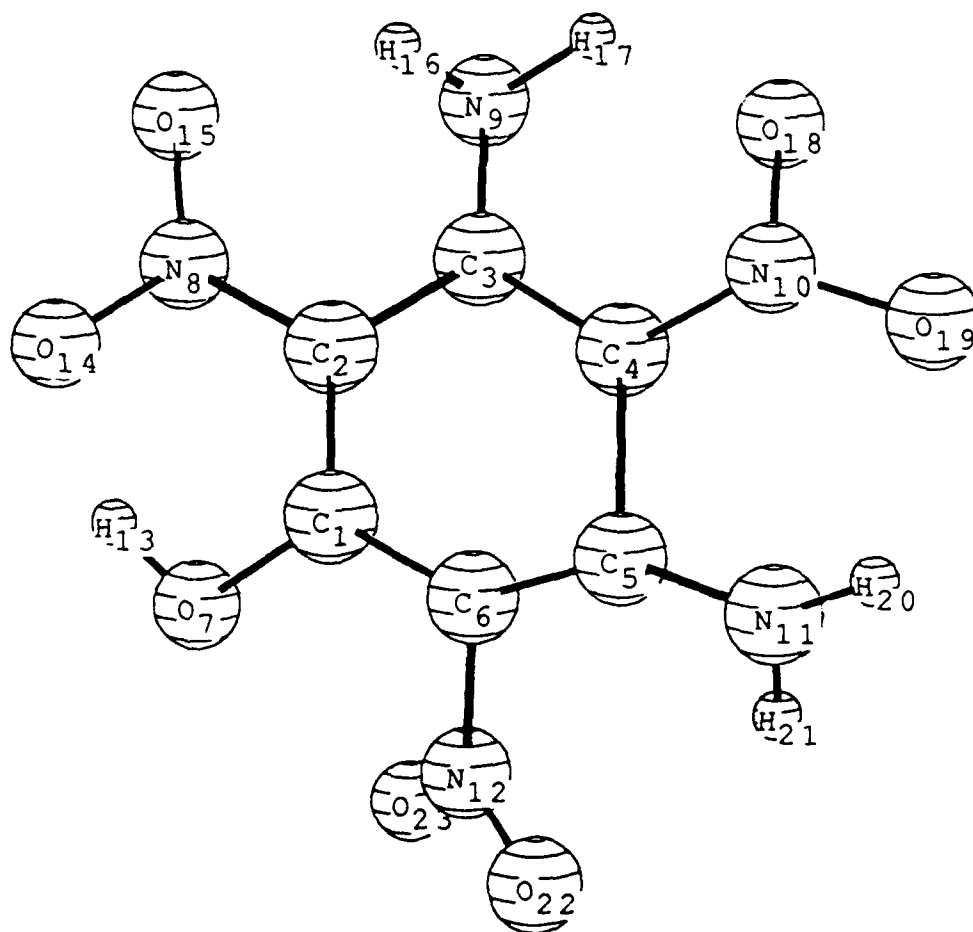


Figure S-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dichloro-2,4,6-trinitroanisole, in the plane 1.75 Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX T
3,5-DIAMINO-2,4,6-TRINITROPHENOL

The short distances between non-bonded hydrogens and oxygens (suggesting hydrogen bonding) are between H13-O14 (1.60 Å), H16-O15 (1.95 Å), H17-O18 (1.76 Å) and H20-O19 (2.05 Å).

The N8 nitro group is rotated by about 5°, the N10 nitro group is rotated by about 13°, and the N12 nitro group is out of the plane by almost 55°. Both the amine groups are rotated by approximately 16°.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.413954 (1)					
3	3	C	2	1.443178 (2)	1	120.438 (23)			
4	4	C	3	1.434645 (3)	2	117.374 (24)	1	-8.553 (44)	0
5	5	C	4	1.436577 (4)	3	121.930 (25)	2	1.239 (45)	0
6	6	C	5	1.421232 (5)	4	115.788 (26)	3	8.545 (46)	0
7	7	O	1	1.332665 (6)	2	123.188 (27)	3	-177.912 (47)	0
8	8	N	2	1.408724 (7)	3	120.150 (28)	4	173.575 (48)	0
9	9	N	3	1.320210 (8)	4	120.822 (29)	5	179.712 (49)	0
10	10	N	4	1.423957 (9)	5	118.620 (30)	6	-172.299 (50)	0
11	11	N	5	1.313367 (10)	6	120.493 (31)	1	169.219 (51)	0
12	12	N	6	1.462077 (11)	1	116.831 (32)	2	-175.794 (52)	0
13	13	H	7	1.016321 (12)	1	102.680 (33)	2	12.438 (53)	0
14	14	O	8	1.277081 (13)	2	119.021 (34)	3	-174.636 (54)	0
15	15	O	8	1.239608 (14)	2	123.042 (35)	3	3.770 (55)	0
16	16	H	9	0.868088 (15)	3	119.640 (36)	4	-162.508 (56)	0
17	17	H	9	1.100023 (16)	3	118.634 (37)	4	-15.787 (57)	0
18	18	O	10	1.247178 (17)	4	120.094 (38)	5	167.570 (58)	0
19	19	O	10	1.247503 (18)	4	120.066 (39)	5	-12.472 (59)	0
20	20	H	11	0.863344 (19)	5	130.140 (40)	6	-167.718 (60)	0
21	21	H	11	0.772446 (20)	5	121.659 (41)	6	16.534 (61)	0
22	22	O	12	1.236374 (21)	6	117.596 (42)	1	-128.339 (62)	0
23	23	O	12	1.208878 (22)	6	118.298 (43)	1	54.347 (63)	0

STOICHIOMETRY C6H5N5O7

EIGENVALUES — -0.29164 0.12482 0.14899 0.18960 0.24369

Estimated ionization potential: 7.95 ev

TOTAL ATOMIC CHARGES.			<u>Net Charges</u>	
		1		
1	C	5.787545	C1	+0.212
2	C	6.018021	C2	-0.018
3	C	5.775208	C3	0.225
4	C	5.997978	C4	0.002
5	C	5.745618	C5	0.254
6	C	5.997326	C6	0.003
7	O	8.291952	O7	-0.292
8	N	6.854899	N8	0.145
9	N	7.471661	N9	-0.472
10	N	6.848168	N10	0.152
11	N	7.609589	N11	-0.610
12	N	6.830704	N12	0.169
13	H	0.714630	H13	0.285
14	O	8.236545	O14	-0.237
15	O	8.179622	O15	-0.180
16	H	0.715319	H16	0.295
17	H	0.729627	H17	0.270
18	O	8.226027	O18	-0.226
19	O	8.226027	O19	-0.207
20	H	0.681906	H20	0.318
21	H	0.675475	H21	0.325
22	O	8.221878	O22	-0.222
23	O	8.183565	O23	-0.184

DIPOLE MOMENT (DEBYE): X= 1.4000 Y=-0.6843 Z= 2.4128 TOTAL= 2.8723

V-mid: N8-C2: 0.095
V-mid: N10-C4: 0.114
V-mid: N12-C6: 0.125

Bond Order: N8-C2: 1.41
Bond Order: N10-C4: 1.36
Bond Order: N12-C6: 1.26
Bond Order: O14-N8: 1.69
Bond Order: O15-N8: 1.85
Bond Order: O18-N10: 1.82
Bond Order: O19-N10: 1.82
Bond Order: O22-N12: 1.86
Bond Order: O23-N12: 1.99

0.0000
 -25.1004
 -12.5502
 - 9.4126
 - 6.2751
 - 3.1376
 - 2.8238
 - 2.5100
 - 2.1963
 - 1.8825
 - 1.2550
 0.6275
 0.6275
 1.8825
 3.1376
 5.0201
 6.2751
 9.4126
 12.5502
 31.3755
 50.2007
 62.7509

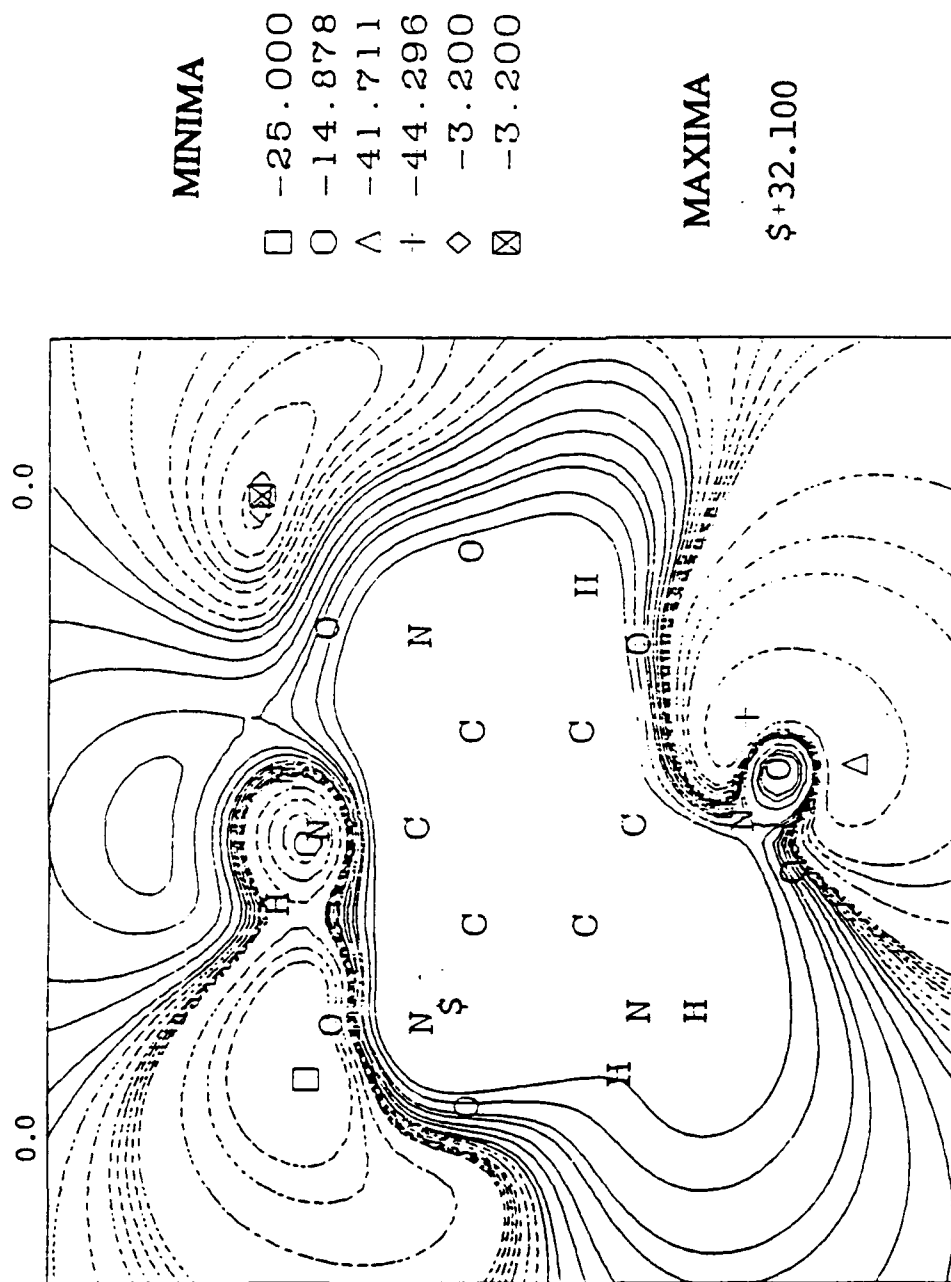
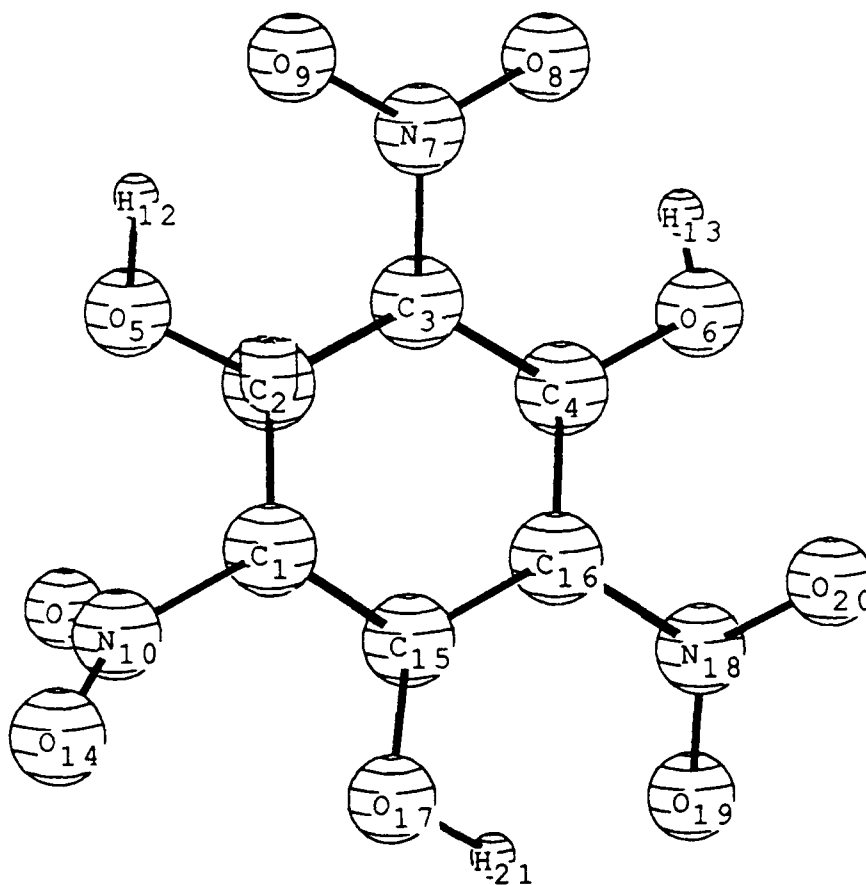


Figure T-1. Calculated electrostatic potential, in kcal/mole, of 3,5-diamino-2,4,6-trinitrophenol, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX U
2,4,6-TRINITROPHLOROGLUCINOL

The short distances between non-bonded hydrogens and oxygens are H13-O8 (1.73 Å), H12-O9 (1.73 Å), and H21-O19 (1.74 Å).

The N7 and N18 nitro groups are rotated out of the plane of the benzene ring by only a few degrees, while the N10 nitro group is rotated by approximately 63°.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA J
1	1	C						
2	2	C	1	1.386018 (1)				
3	3	C	2	1.410857 (2)	1	118.233 (21)		
4	4	C	3	1.415998 (3)	2	120.706 (22)	1	2.096 (40) 0
5	5	O	2	1.326719 (4)	3	124.750 (23)	4	-178.414 (41) 0
6	6	O	4	1.310592 (5)	3	120.643 (24)	2	178.934 (42) 0
7	7	N	3	1.436206 (6)	2	119.229 (25)	1	-175.048 (43) 0
8	8	O	7	1.227657 (7)	3	120.519 (26)	2	-176.095 (44) 0
9	9	O	7	1.240487 (8)	3	118.609 (27)	2	4.684 (45) 0
10	10	N	1	1.466242 (9)	2	118.321 (28)	3	178.961 (46) 0
11	11	O	10	1.221284 (10)	1	117.732 (29)	2	62.714 (47) 0
12	12	H	5	0.991694 (11)	2	112.087 (30)	3	-14.216 (48) 0
13	13	H	4	1.767937 (12)	3	93.388 (31)	2	178.073 (49) 0
14	14	O	10	1.221284 (13)	1	117.732 (32)	2	-117.286 (50) 0
15	15	C	1	1.386018 (14)	10	118.321 (33)	14	62.714 (51) 0
16	16	C	15	1.410857 (15)	1	118.233 (34)	10	-178.961 (52) 0
17	17	O	15	1.326719 (16)	16	124.750 (35)	4	-178.414 (53) 0
18	18	N	16	1.436206 (17)	15	119.229 (36)	1	-175.048 (54) 0
19	19	O	18	1.240487 (18)	16	118.609 (37)	15	4.684 (55) 0
20	20	O	18	1.227657 (19)	16	120.519 (38)	15	-176.095 (56) 0
21	21	H	17	0.991694 (20)	15	112.087 (39)	16	-14.216 (57) 0

STOICHIOMETRY C6H3N3O9

E=1061.04187210

EIGENVALUES — -0.28887 0.10982 0.13449 0.19142 0.23070

Estimated ionization potential: 7.9 ev

TOTAL ATOMIC CHARGES.

		1	<u>Net Charges</u>
1	C	5.980876	+0.02
2	C	5.776130	+0.22
3	C	6.021020	-0.02
4	C	5.762782	+0.24
5	O	8.295881	-0.30
6	O	8.342514	-0.34
7	N	6.829723	+0.17
8	O	8.203208	-0.20
9	O	8.209679	-0.21
10	N	6.820550	+0.18
11	O	8.191891	-0.19
12	H	0.705208	+0.29
13	H	0.665175	+0.33
14	O	8.190493	-0.19
15	C	5.775829	+0.22
16	C	5.998390	0.00
17	O	8.295988	-0.30
18	N	6.834414	+0.17
19	O	8.246792	-0.25
20	O	8.152027	-0.15
21	H	0.701428	+0.30

DIPOLE MOMENT (DEBYE): X= 1.4101 Y=-0.0146 Z= 2.5837 TOTAL= 2.9435

V_{mid}: C₁-N₁₀: 0.143
 C₃-N₇: 0.110
 C₁₆-N₁₈: 0.123

Bond Orders: C₁-N₁₀: 1.26 N₇-O₉: 1.99
 C₃-N₇: 1.34 N₁₈-O₁₉: 1.99
 C₁₆-N₁₈: 1.34 N₁₈-O₂₀: 2.05
 N₁₀-O₁₁: 2.09
 N₁₀-O₁₄: 2.09
 N₇-O₈: 2.05

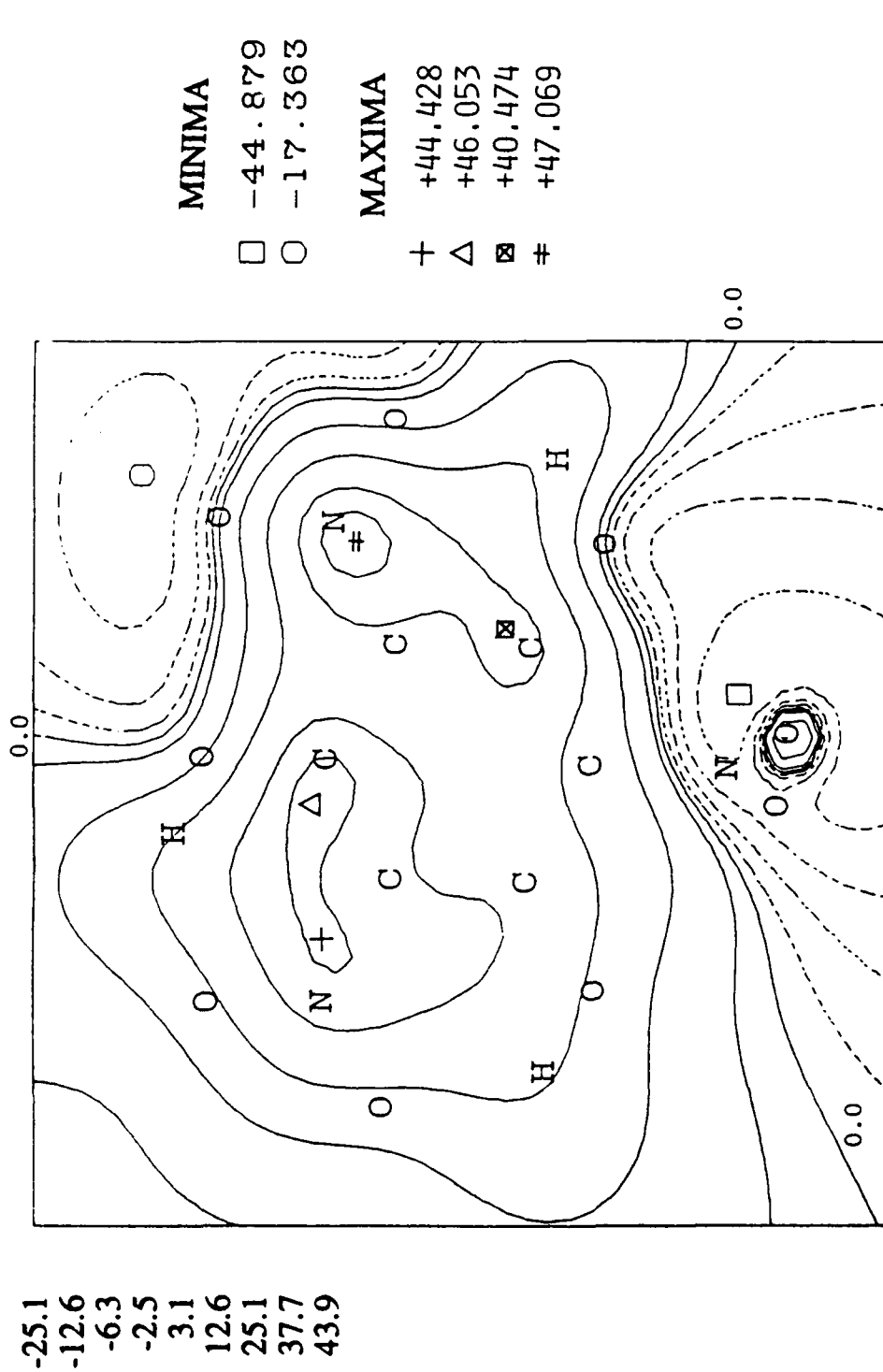
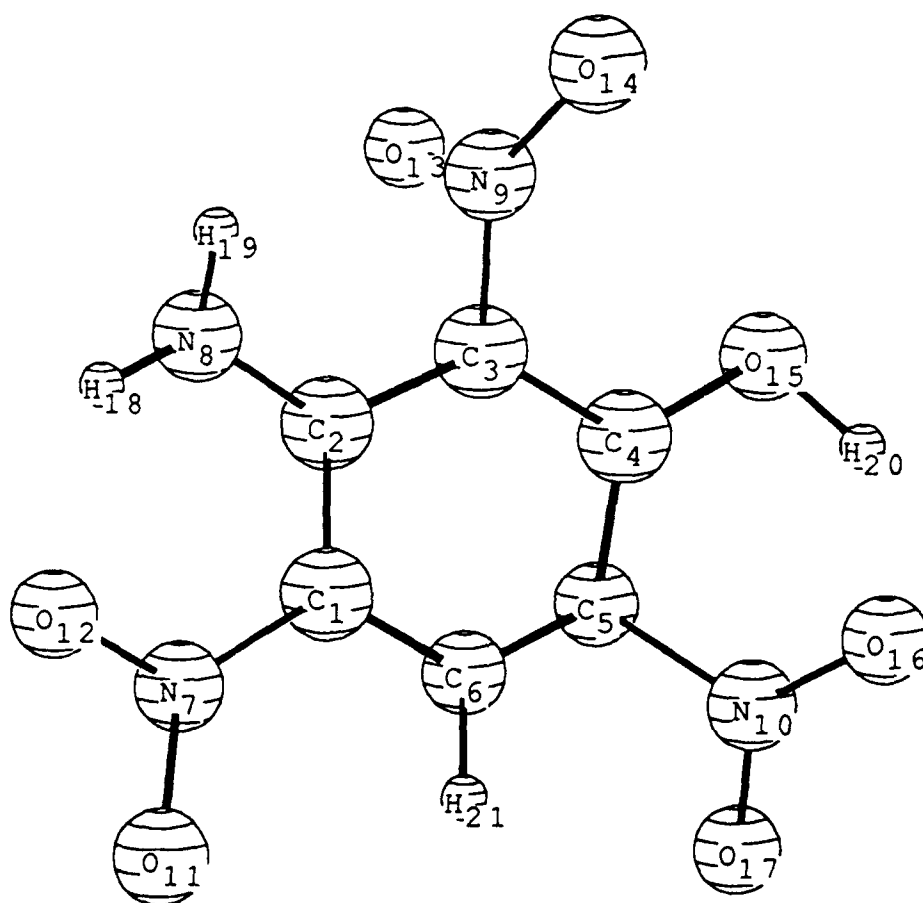


Figure U-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrophenol, in the plane 1.75Å above the N18 nitro group located in the upper right corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX V AMINOPICRIC ACID

The short distances between non-bonded hydrogens and oxygens strongly suggest hydrogen bonding within the molecule. These are between H21-O17 (2.33 Å), H18-O12 (1.96 Å), H19-O13 (2.02 Å), H21-O11 (2.35 Å), and H20-O16 (1.65 Å).

The N7 nitro group is almost planar with the mean plane of the benzene ring, but the N9 nitro group is out of the plane by about 43° and the N10 nitro group is out of the plane by about 4°. The amine group (N8) is essentially planar.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CONT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.425800 (1)					
3	3	C	2	1.416065 (2)	1	114.909 (21)			
4	4	C	3	1.394424 (3)	2	124.307 (22)	1	0.780 (40)	0
5	5	C	4	1.411584 (4)	3	116.911 (23)	2	2.197 (41)	0
6	6	C	5	1.374855 (5)	4	120.888 (24)	3	-3.555 (42)	0
7	7	N	1	1.457638 (6)	2	121.380 (25)	3	176.949 (43)	0
8	8	N	2	1.315976 (7)	3	121.291 (26)	4	179.606 (44)	0
9	9	N	3	1.466324 (8)	4	116.004 (27)	5	179.897 (45)	0
10	10	N	5	1.439569 (9)	6	117.313 (28)	1	179.668 (46)	0
11	11	O	7	1.221251 (10)	1	118.353 (29)	2	-178.866 (47)	0
12	12	O	7	1.226672 (11)	1	119.170 (30)	2	0.351 (48)	0
13	13	O	9	1.227247 (12)	3	117.678 (31)	4	136.705 (49)	0
14	14	O	9	1.213759 (13)	3	119.079 (32)	4	-43.446 (50)	0
15	15	O	4	1.336226 (14)	5	123.609 (33)	6	178.929 (51)	0
16	16	O	10	1.244771 (15)	5	118.211 (34)	6	-175.804 (52)	0
17	17	O	10	1.209722 (16)	5	113.526 (35)	6	4.846 (53)	0
18	18	H	8	0.900000 (17)	2	119.800 (36)	3	-178.200 (54)	0
19	19	H	8	0.900000 (18)	2	113.100 (37)	3	-3.540 (55)	0
20	20	H	15	1.150000 (19)	4	108.200 (38)	5	-16.100 (56)	0
21	21	H	6	0.970000 (20)	5	118.000 (39)	4	186.000 (57)	0

STOICHIOMETRY C6H4N4O7

.....
SCF DONE: E(RHF) = -966.795803082 A.U. AFTER 29 CYCLES
.....

EIGENVALUES — -0.30622 -0.30542 0.12646 0.14052 0.18294

Estimated ionization potential: 8.31 ev

TOTAL ATOMIC CHARGES

		1	Net Charges
1	C	5.962634	+0.04
2	C	5.776352	+0.22
3	C	5.982033	+0.02
4	C	5.795539	+0.20
5	C	5.979536	+0.02
6	C	6.030805	-0.03
7	N	6.829224	+0.17
8	N	7.515466	-0.52
9	N	6.831797	+0.17
10	N	6.824527	+0.18
11	O	8.192717	-0.19
12	O	8.226350	-0.23
13	O	8.224539	-0.22
14	O	8.174667	-0.17
15	O	8.268007	-0.27
16	O	8.238083	-0.24
17	O	8.156888	-0.16
18	H	0.697097	+0.30
19	H	0.714770	+0.29
20	H	0.727397	+0.27
21	H	0.851573	+0.15

DIPOLE MOMENT (DEBYE): X=-0.3363 Y=-0.5848 Z=-0.1270 TOTAL= 0.6864

V-mid N7-C1: 0.151
 N9-C3: 0.134
 N10-C5: 0.143

Bond Orders:

C1-N7: 1.27
 C2-N8: 1.71
 C3-N9: 1.25
 C5-N10: 1.32
 N7-O11: 1.95
 N7-O12: 1.90
 N9-O13: 1.90
 N9-O14: 2.00
 N10-O16: 1.86
 N10-O17: 2.00

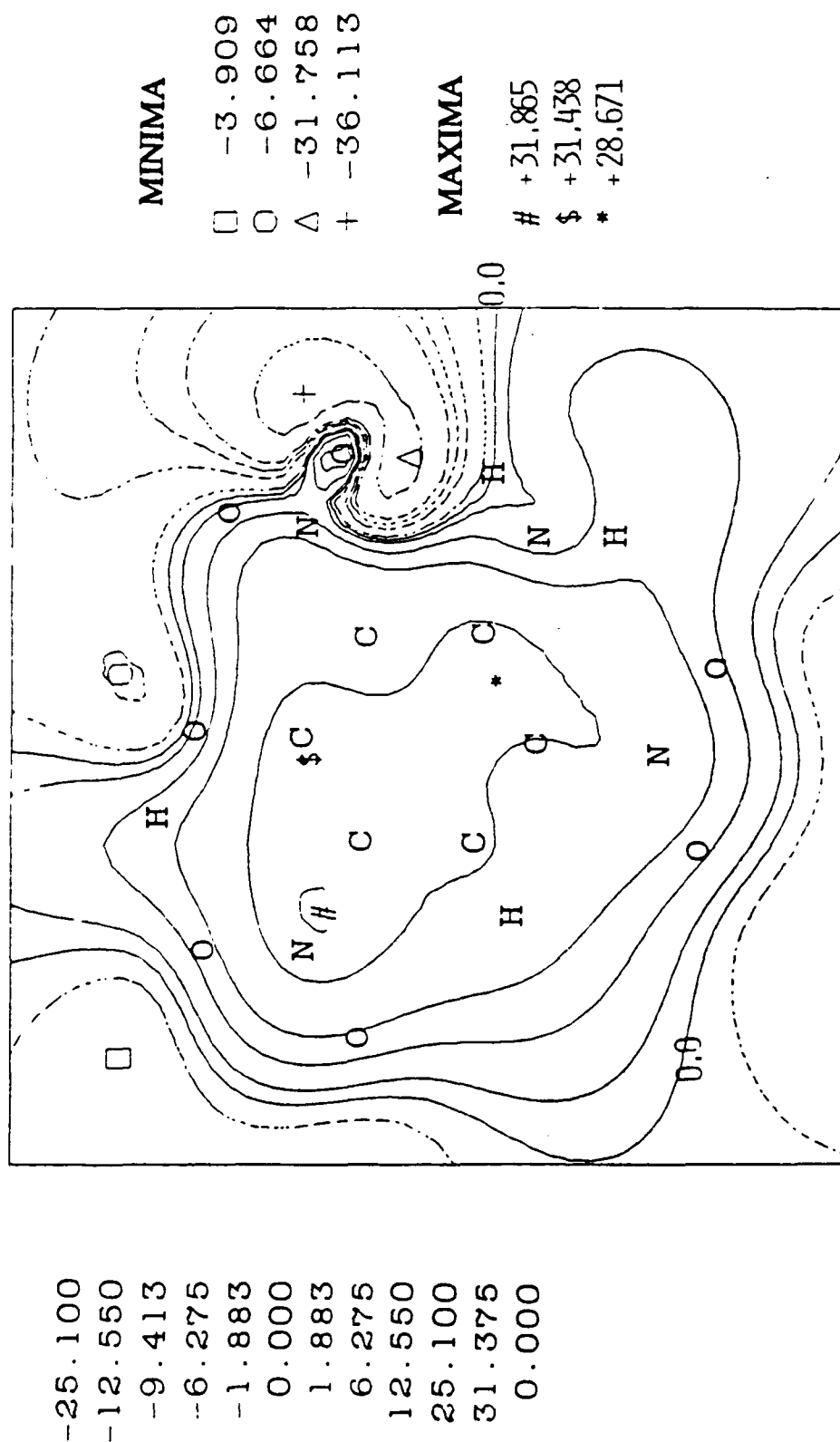


Figure V-1. Calculated electrostatic potential, in kcal/mole, of aminopicric acid, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

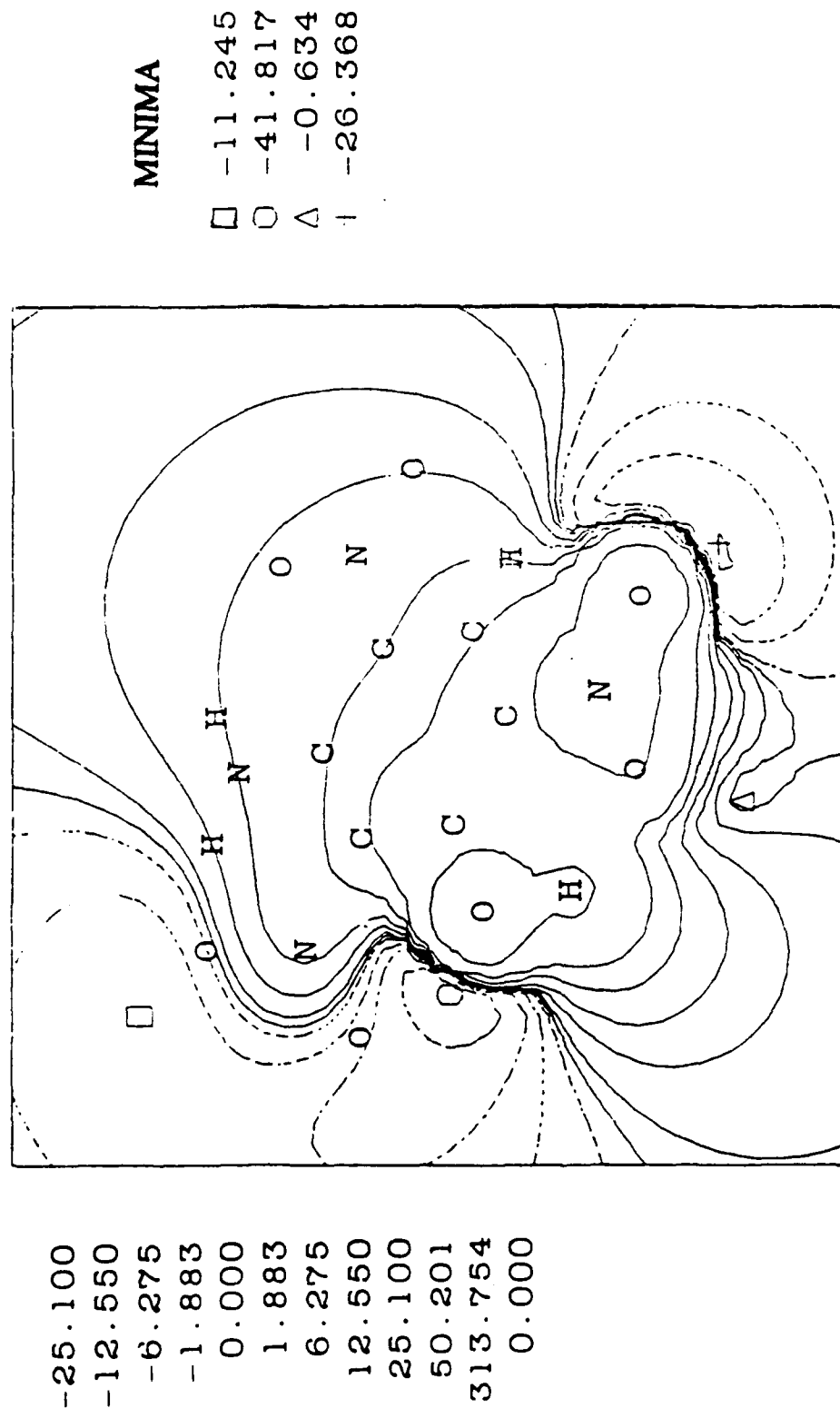
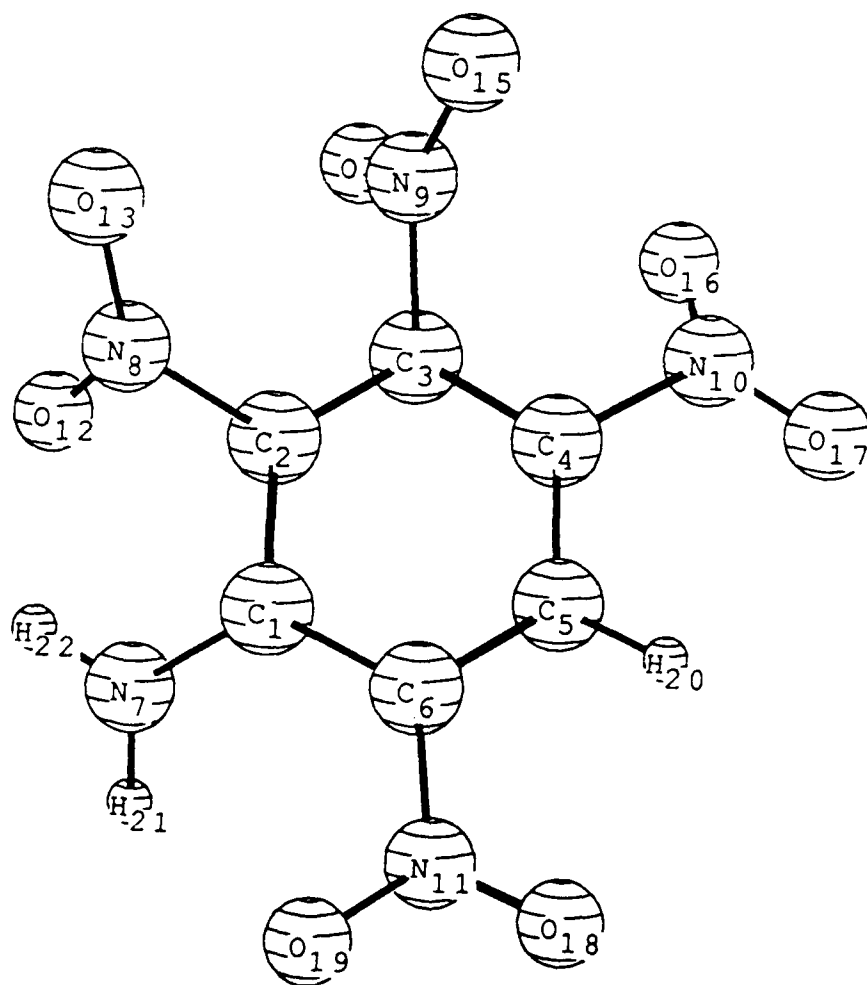


Figure V-2. Calculated electrostatic potential, in kcal/mole, of aminopicric acid, in the plane 1.75 Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX W
2,3,4,6-TETRANITROANILINE

The short distances between non-bonded hydrogens and oxygens are between H22-O12 (2.03Å), H20-O17 (2.32 Å), H20-O18 (2.36Å) and H21-O19 (1.95Å).

The N11 nitro group is approximately coplanar with the ring. The nitro groups N8, N9, N10 are rotated approximately, 45°, 65°, and 14° respectively. The amine group is almost planar.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.434000 (1)					
3	3	C	2	1.361000 (2)	1	122.000 (22)			
4	4	C	3	1.384000 (3)	2	120.000 (23)	1	-0.950 (42)	0
5	5	C	4	1.377000 (4)	3	120.750 (24)	2	-2.930 (43)	0
6	6	C	1	1.428000 (5)	2	115.000 (25)	3	4.790 (44)	0
7	7	N	1	1.312000 (6)	2	122.000 (26)	3	-176.000 (45)	0
8	8	N	2	1.467000 (7)	3	119.000 (27)	4	174.000 (46)	0
9	9	N	3	1.487000 (8)	2	118.000 (28)	1	-179.000 (47)	0
10	10	N	4	1.447000 (9)	3	122.000 (29)	2	172.000 (48)	0
11	11	N	6	1.461000 (10)	1	122.000 (30)	2	177.000 (49)	0
12	12	O	8	1.218000 (11)	2	118.000 (31)	1	-45.000 (50)	0
13	13	O	8	1.218000 (12)	2	117.000 (32)	1	133.000 (51)	0
14	14	O	9	1.211000 (13)	3	116.000 (33)	2	-65.000 (52)	0
15	15	O	9	1.207000 (14)	3	116.000 (34)	2	114.980 (53)	0
16	16	O	10	1.221000 (15)	4	118.000 (35)	3	-14.000 (54)	0
17	17	O	10	1.227000 (16)	4	118.000 (36)	3	165.000 (55)	0
18	18	O	11	1.215000 (17)	6	119.000 (37)	1	-179.000 (56)	0
19	19	O	11	1.222000 (18)	6	118.000 (38)	1	-10.000 (57)	0
20	20	H	5	1.020000 (19)	4	117.000 (39)	3	-179.000 (58)	0
21	21	H	7	0.950000 (20)	1	120.000 (40)	2	177.000 (59)	0
22	22	H	7	0.970000 (21)	1	119.000 (41)	2	5.640 (60)	0

STOICHIOMETRY C6H3N5O8

.....
 SCF DONE: E(RHF) = -1094.81498704 A.U. AFTER 36 CYCLES

EIGENVALUES — -0.33140 -0.32703 -0.32170 -0.31199 0.09964

Estimated ionization potential: 8.49 ev

TOTAL ATOMIC CHARGES:

	1	Net Charges
1 C	5.781556	+0.22
2 C	5.940497	+0.06
3 C	5.863175	+0.14
4 C	5.932056	+0.07
5 C	6.020843	-0.02
6 C	5.944619	+0.06
7 N	7.466881	-0.47
8 N	6.822964	+0.18
9 N	6.796636	+0.20
10 N	6.830082	+0.17
11 N	6.824287	+0.18
12 O	8.203361	-0.20
13 O	8.171323	-0.17
14 O	8.177237	-0.17
15 O	8.162989	-0.16
16 O	8.189204	-0.19
17 O	8.194223	-0.19
18 O	8.180426	-0.18
19 O	8.219833	-0.22
20 H	0.843741	+0.16
21 H	0.709041	+0.29
22 H	0.725024	+0.27

DIPOLE MOMENT (DEBYE): X=-2.4264 Y= 0.5727 Z=-4.1587 TOTAL= 4.8487

V-mid: N8-C2: 0.172
 N9-C3: 0.236
 N10-C4: 0.174
 N11-C6: 0.170

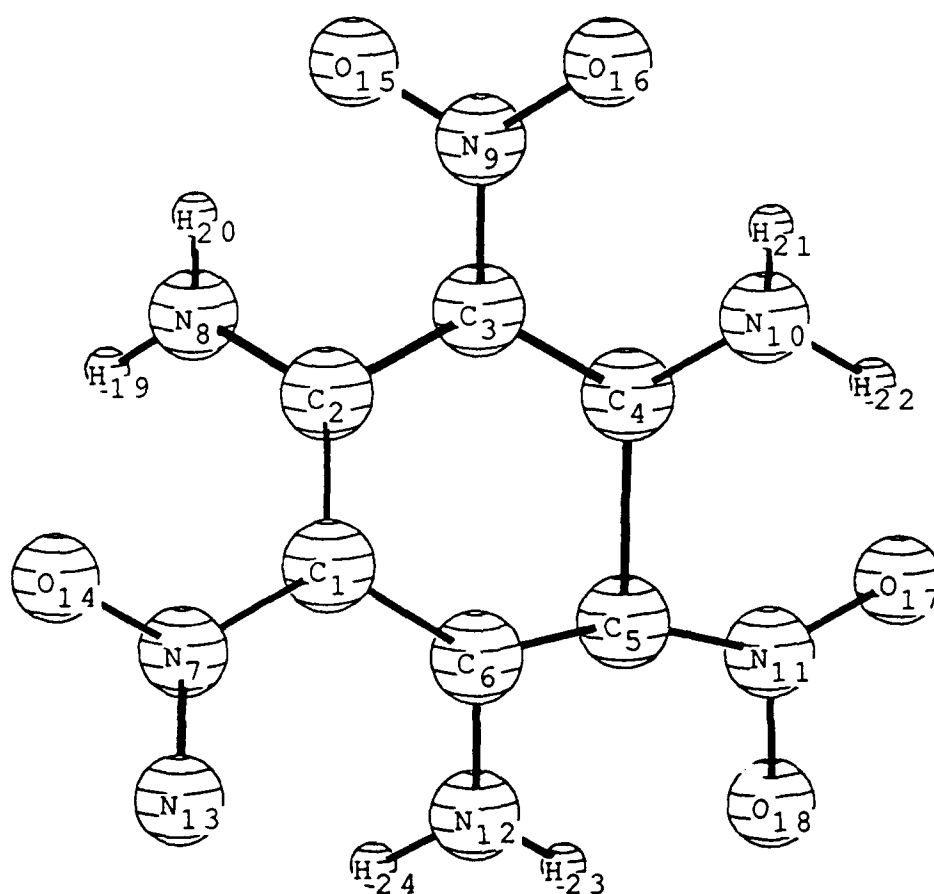
Bond Orders:

C1-N7: 1.74
 C2-N8: 1.24
 C3-N9: 1.20
 C4-N10: 1.30
 C6-N11: 1.26

 N8-O12: 1.96
 N8-O13: 1.96
 N9-O14: 2.00
 N9-O15: 2.02
 N10-O16: 1.95
 N10-O17: 1.92
 N11-O18: 1.98
 N11-O19: 1.94

APPENDIX X
1,3,5-TRIAMINO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are between H21-O16 (1.95Å), H22-O18 (1.69Å), H23-O19 (1.82Å), H19-O14 (1.80Å), H20-O15 (1.84Å), and H24-O13 (1.77Å). All nitro groups are essentially coplanar.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.435000 (1)					
3	3	C	2	1.447835 (2)	1	117.958 (24)			
4	4	C	3	1.436690 (3)	2	121.823 (25)	1	1.563 (46)	0
5	5	C	4	1.445519 (4)	3	117.995 (26)	2	2.699 (47)	0
6	6	C	5	1.435637 (5)	4	122.258 (27)	3	-5.062 (48)	0
7	7	N	1	1.416866 (6)	2	119.178 (28)	3	176.375 (49)	0
8	8	N	2	1.308986 (7)	3	120.727 (29)	4	-177.599 (50)	0
9	9	N	3	1.416524 (8)	4	119.045 (30)	5	-177.489 (51)	0
10	10	N	4	1.318790 (9)	5	120.543 (31)	6	175.500 (52)	0
11	11	N	5	1.422453 (10)	6	119.115 (32)	1	-178.785 (53)	0
12	12	N	6	1.310130 (11)	1	121.122 (33)	2	-177.498 (54)	0
13	13	O	7	1.235980 (12)	1	121.326 (34)	2	-178.209 (55)	0
14	14	O	7	1.242231 (13)	1	120.766 (35)	2	3.156 (56)	0
15	15	O	9	1.245843 (14)	3	120.644 (36)	4	177.655 (57)	0
16	16	O	9	1.238782 (15)	3	121.489 (37)	4	-1.816 (58)	0
17	17	O	11	1.243651 (16)	5	121.325 (38)	6	-179.192 (59)	0
18	18	O	11	1.251906 (17)	5	121.000 (39)	6	-1.683 (60)	0
19	19	H	8	0.864445 (18)	2	117.278 (40)	3	179.362 (61)	0
20	20	H	8	0.848948 (19)	2	119.427 (41)	3	-13.477 (62)	0
21	21	H	10	0.756530 (20)	4	123.058 (42)	5	175.709 (63)	0
22	22	H	10	1.054022 (21)	4	120.725 (43)	5	1.598 (64)	0
23	23	H	12	0.868277 (22)	6	119.010 (44)	1	177.745 (65)	0
24	24	H	12	0.954518 (23)	6	116.561 (45)	1	13.077 (66)	0

STOICHIOMETRY C6H6N6O6

.....
SCF DONE: E(RHF) = -1001.76753338 A.U. AFTER 29 CYCLES
.....

EIGENVALUES — -0.28957 0.14706 0.15303 0.17304 0.26932

Estimated ionization potential: 7.9 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	6.016830	-0.02
2	C	5.752293	+0.25
3	C	6.014397	-0.01
4	C	5.755384	+0.24
5	C	6.015664	-0.02
6	C	5.761298	+0.24
7	N	6.843190	+0.16
8	N	7.567198	-0.57
9	N	6.849386	+0.15
10	N	7.558035	-0.56
11	N	6.845056	+0.15
12	N	7.519123	-0.52
13	O	8.226725	-0.23
14	O	8.225928	-0.23
15	O	8.233159	0.23
16	O	8.220555	-0.22
17	O	8.227047	-0.23
18	O	8.218506	-0.22
19	H	0.687027	+0.31
20	H	0.683115	+0.32
21	H	0.672935	+0.33
22	H	0.705543	+0.29
23	H	0.694585	+0.31
24	H	0.706062	+0.29

DIPOLE MOMENT (DEBYE): X= 0.3195 Y= 0.2801 Z=-0.6508 TOTAL= 0.7773

V-mid: N7-C1: 0.105
 N9-C3: 0.102
 N11-C5: 0.103

Bond Orders: N7-C1: 1.38
 N8-C2: 1.76
 N9-C3: 1.38
 N10-C4: 1.72
 N11-C5: 1.37
 N12-C6: 1.75
 N7-O13: 1.86
 N7-O14: 1.84
 N9-O15: 1.82
 N9-O16: 1.85
 N11-O17: 1.83
 N11-O18: 1.79

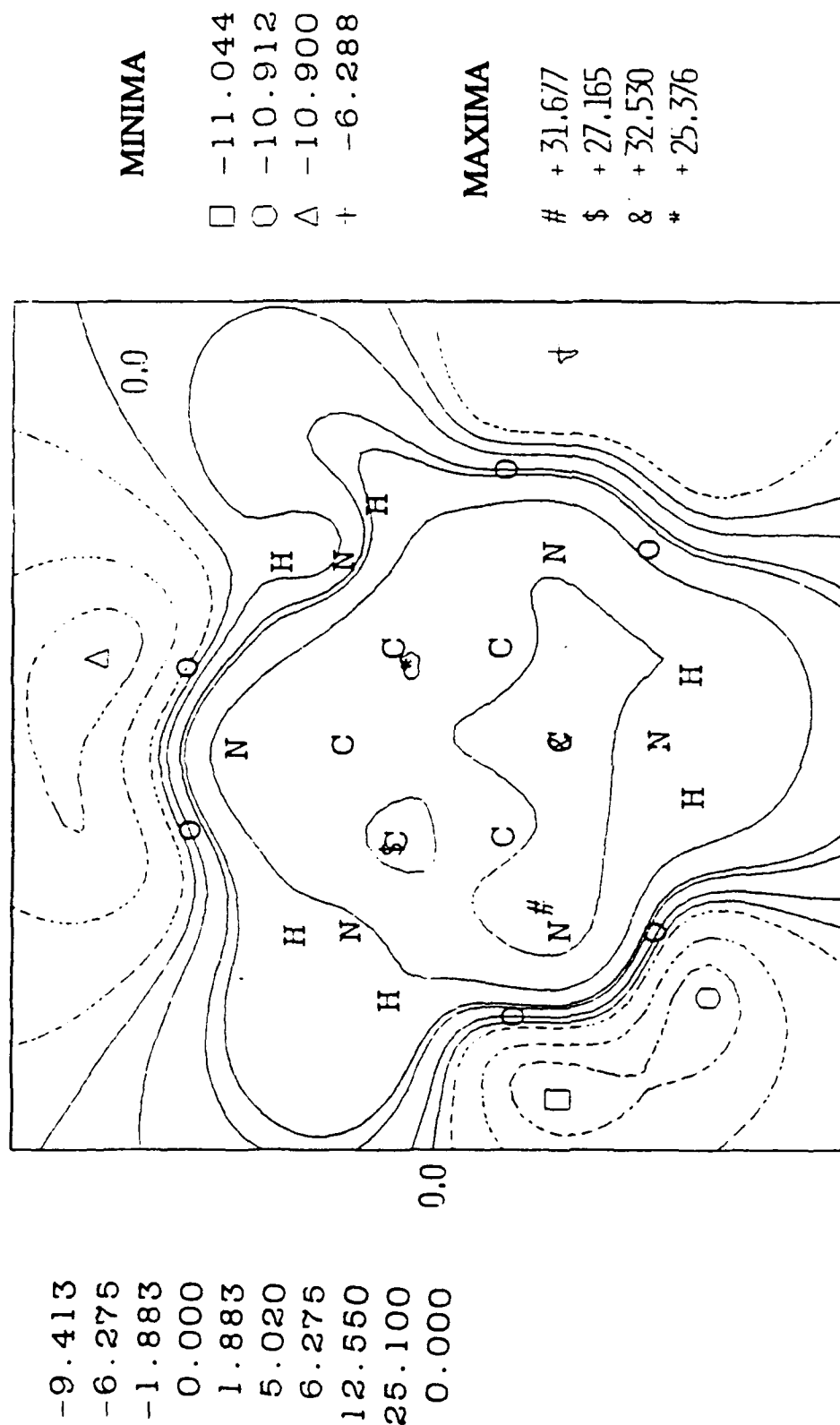
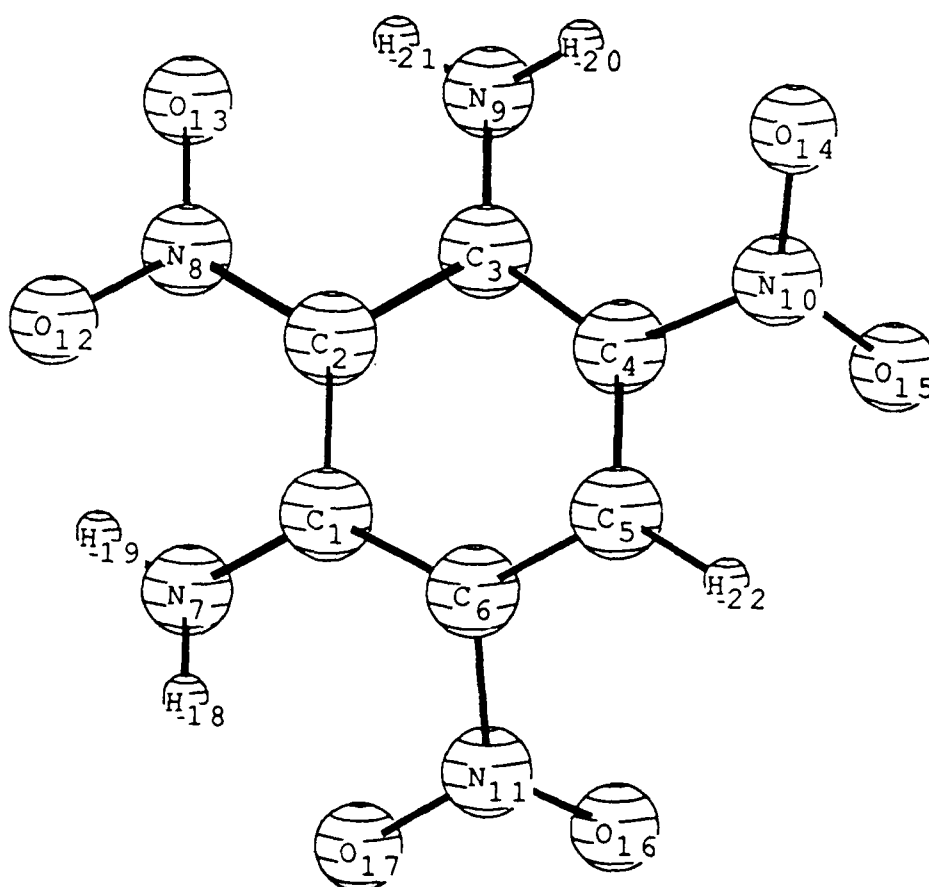


Figure X-1. Calculated electrostatic potential, in kcal/mole, of 1,3,5-triamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are indicated. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Y
1,3-DIAMINO-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H21-O16 (1.95 Å), H22-O18 (1.69 Å), H23-O19 (1.82 Å), H19-O14 (1.80 Å), H20-O15 (1.84 Å) and H24 - O13 (1.77 Å).

All nitro groups and amine groups are essentially coplanar.



Z-Matrix (Angstroms and Degrees)							
Cent	Atom	N1	Length	N2	Alpha	N3	Beta
1	C						
2	C	1	1.4664356				
3	C	2	1.4723277	1	120.5247574		
4	C	3	1.3918228	2	115.8793259	1	-4.2251754
5	C	4	1.3789175	3	123.8528214	2	4.0671515
6	C	5	1.3739673	4	119.2582703	3	-3.1503119
7	N	1	1.3228761	6	124.0092850	5	179.7978668
8	N	2	1.4151319	1	119.6532745	6	-178.1909485
9	N	3	1.3177489	2	120.1124573	1	177.7904205
10	N	4	1.4318832	3	122.4196014	2	-179.6103363
11	N	6	1.5139433	1	121.9566345	2	-177.3157349
12	O	8	1.2621572	2	121.7608109	3	-178.2516937
13	O	8	1.2413824	2	120.8816833	3	-1.2636397
14	O	10	1.2597437	4	118.7223892	5	-174.9521942
15	O	10	1.2230211	4	121.2245178	5	1.6063229
16	O	11	1.1772938	6	117.8368988	1	173.3712616
17	O	11	1.2357228	6	115.5550537	1	-8.5564947
18	H	7	0.8897375	1	119.3610306	2	-179.9651947
19	H	7	0.8905061	1	119.2657166	2	0.0104214
20	H	9	0.8902898	3	119.2623444	4	2.1553166
21	H	9	0.8901286	3	119.3083496	4	-177.8555298
22	H	5	1.0802929	6	120.2810669	1	-177.6110077

Stoichiometry: C6H5N5O6

SCF DONE: E(RHF) = -947.084610

EIGENVALUES -- -0.29970 -.29735 0.12008 .15933 0.18091

Estimated ionization potential: 8.09 ev

TOTAL ATOMIC CHARGES.

		1
1	C	5.775821
2	C	5.958405
3	C	5.770389
4	C	5.982352
5	C	5.990443
6	C	5.985343
7	N	7.533139
8	N	6.854927
9	N	7.532075
10	N	6.846354
11	N	6.805783
12	O	8.220756
13	O	8.212900
14	O	8.231972
15	O	8.190286
16	O	8.188858
17	O	8.236980
18	H	0.703012
19	H	0.696854
20	H	0.701672
21	H	0.695836
22	H	0.849761

Net Charges

1	C	+ 0.22
2	C	+ 0.01
3	C	+ 0.23
4	C	+ 0.02
5	C	0.00
6	C	+ 0.01
7	N	- 0.53
8	N	+ 0.15
9	N	- 0.53
10	N	+ 0.15
11	N	+ 0.19
12	O	- 0.22
13	O	- 0.21
14	O	- 0.23
15	O	- 0.19
16	O	- 0.18
17	O	- 0.24
18	H	+ 0.30
19	H	+ 0.30
20	H	+ 0.30
21	H	+ 0.30
22	H	+ 0.15

DIPOLE MOMENT (DEBYE): X = 0.4617 Y = 0.9115 Z = 1.0664 TOTAL = 1.4769

V-mid N8-C2: 0.118
 N10-C4: 0.127
 N11-C6: 0.146

Bond Orders:

C1-N7: 1.70
 C2-N8: 1.39
 C3-N9: 1.72
 C4-N10: 1.34
 C6-N11: 1.13
 N8-O12: 1.76
 N8-O13: 1.86
 N10-O14: 1.77
 N10-O15: 1.94
 N11-O16: 2.17
 N12-O17: 1.88

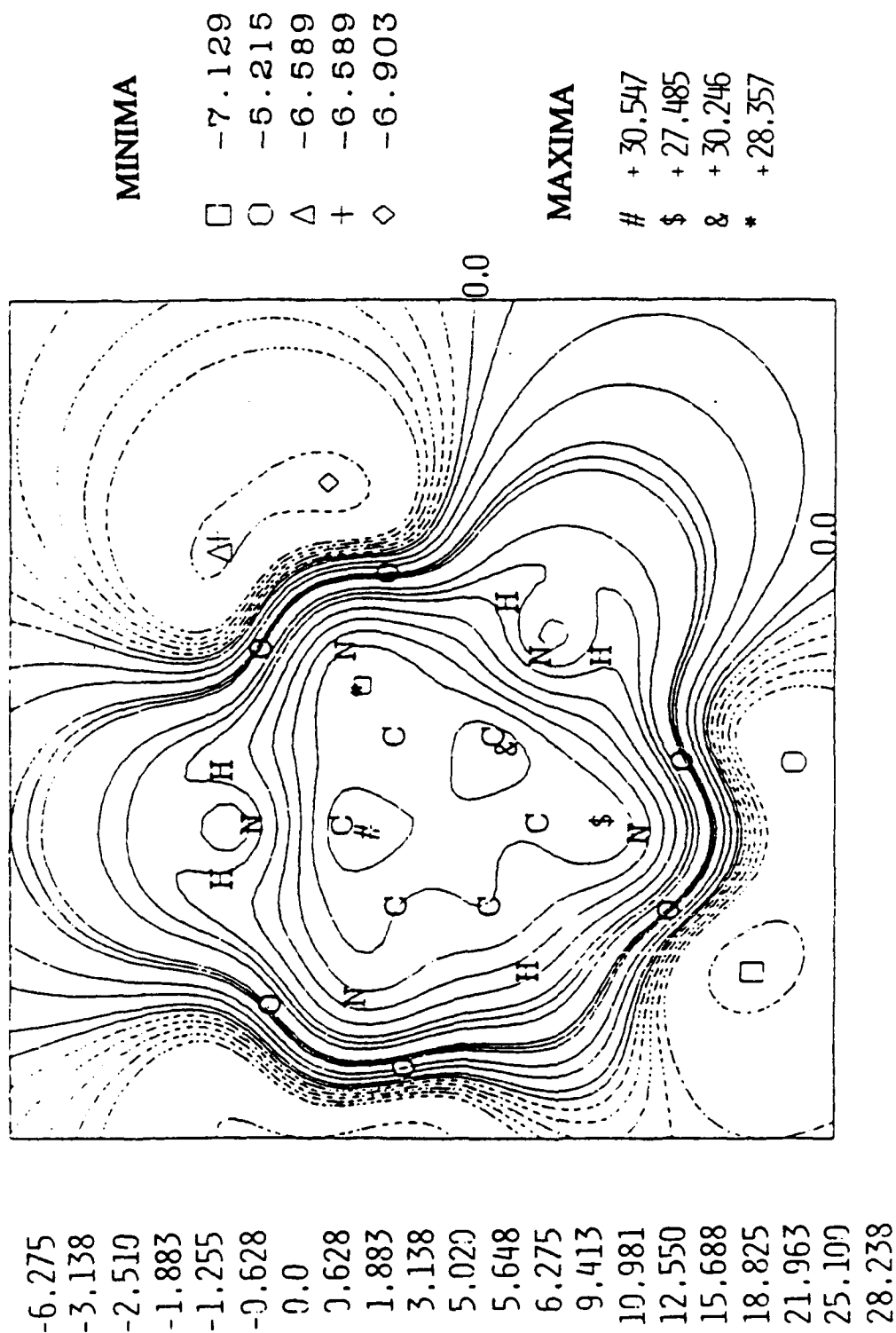
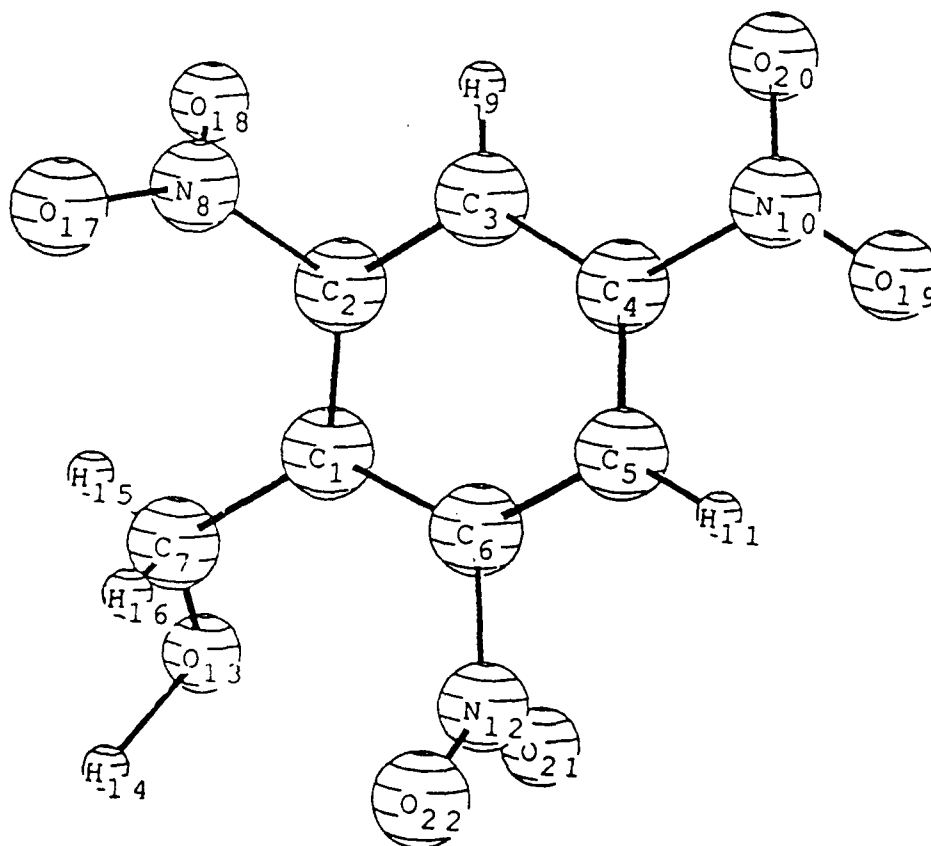


Figure Y-1. Calculated electrostatic potential, in kcal/mole, of 1,3-diamino-2,4,6-trinitrobenzene, in the plane 1.75 Å above the aromatic ring. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX Z
2,4,6-TRINITROBENZYL ALCOHOL

The short distances between non-bonded hydrogens and oxygens are H9-O18 (2.50 Å), H9-O20 (2.45 Å), H11-O19 (2.46 Å) and H15-O17 (2.30 Å).

The N10 nitro group is rotated out of the mean plane of the benzene ring by about 10°, while the N8 and N12 nitro groups are rotated by about 40° and 54°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA
1	1	C						
2	2	C	1	1.357619 (1)				
3	3	C	2	1.372534 (2)	1	125.219 (22)		
4	4	C	3	1.377346 (3)	2	117.473 (23)	1	-0.942 (42) 0
5	5	C	4	1.386211 (4)	3	121.410 (24)	2	0.645 (43) 0
6	6	C	5	1.363131 (5)	4	117.678 (25)	3	-0.079 (44) 0
7	7	C	1	1.499325 (6)	2	124.289 (26)	3	-176.777 (45) 0
8	8	N	2	1.482795 (7)	3	115.382 (27)	4	176.228 (46) 0
9	9	H	3	0.960036 (8)	4	121.412 (28)	5	-179.306 (47) 0
10	10	N	4	1.458971 (9)	5	118.640 (29)	6	175.741 (48) 0
11	11	H	5	0.959774 (10)	6	121.176 (30)	1	179.636 (49) 0
12	12	N	6	1.479611 (11)	1	119.555 (31)	2	176.110 (50) 0
13	13	O	7	1.415276 (12)	1	110.270 (32)	2	136.299 (51) 0
14	14	H	13	1.134622 (13)	7	102.775 (33)	1	146.977 (52) 0
15	15	H	7	0.959596 (14)	1	109.227 (34)	2	18.341 (53) 0
16	16	H	7	0.959905 (15)	1	109.405 (35)	2	-101.570 (54) 0
17	17	C	8	1.196034 (16)	2	118.887 (36)	3	-139.745 (55) 0
18	18	C	8	1.233533 (17)	2	116.414 (37)	3	39.673 (56) 0
19	19	O	10	1.175433 (18)	4	119.343 (38)	5	-9.451 (57) 0
20	20	O	10	1.223853 (19)	4	116.632 (39)	5	168.713 (58) 0
21	21	O	12	1.205410 (20)	6	119.000 (40)	5	-53.936 (59) 0
22	22	O	12	1.230981 (21)	6	116.231 (41)	1	-55.129 (60) 0

STOICHIOMETRY C7H5N3O7

SCF DONE: E(RHF) = -950.841755357

EIGENVALUES — -0.31779 -0.31181 0.11651 0.13601 0.12553

Estimated ionization potential: 8.50 eV

TOTAL ATOMIC CHARGES.

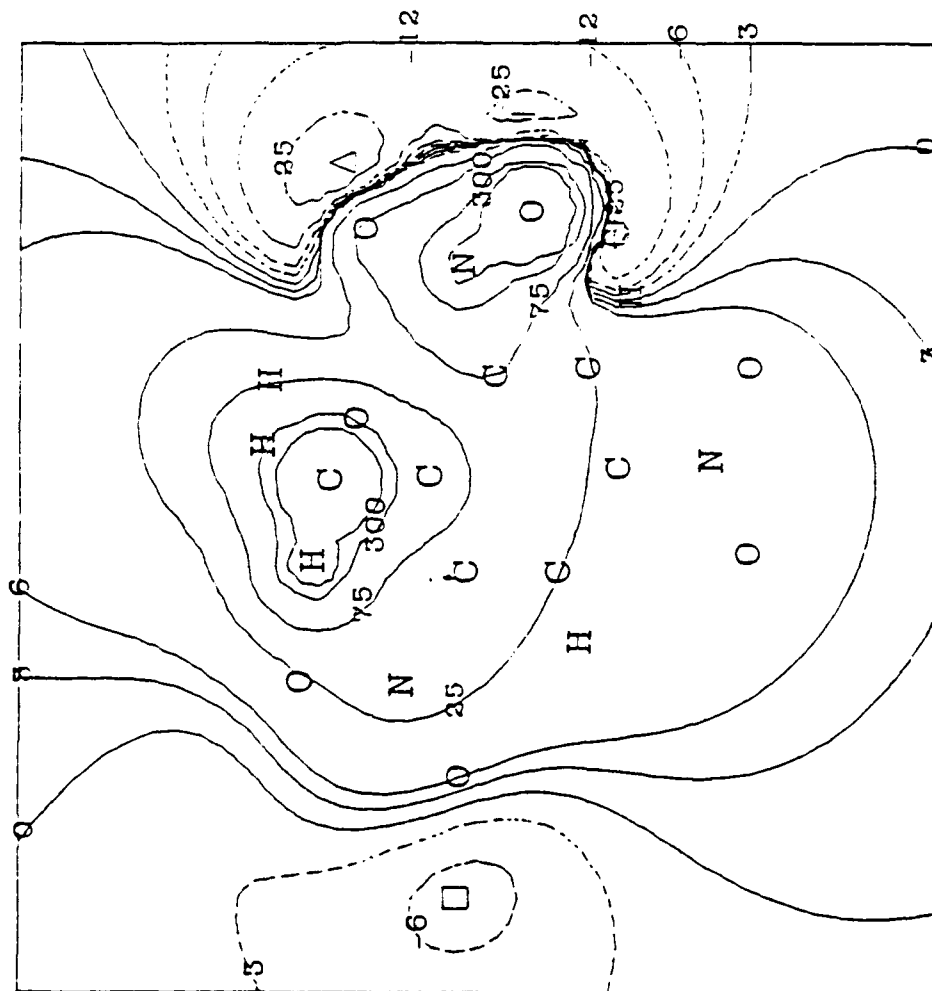
		1	Net Charge
1	C	5.942688	0.057
2	C	5.898740	0.101
3	C	6.061611	-0.062
4	C	5.887629	0.112
5	C	5.065386	-0.107
6	C	5.888654	0.111
7	C	6.082517	-0.083
8	N	6.825415	0.175
9	H	0.252752	0.147
10	N	6.812835	0.187
11	H	0.259317	0.141
12	N	6.819559	0.180
13	O	8.240289	-0.240
14	H	0.837348	0.163
15	H	0.882923	0.117
16	H	0.87624	0.124
17	O	8.190826	-0.190
18	O	8.195151	-0.195
19	O	8.189585	-0.190
20	O	8.205442	-0.205
21	O	8.179062	-0.179
22	O	8.205824	-0.206

DIPOLE MOMENT (DEBYE): X=-1.6231 Y=-0.7876 Z=-0.9997 TOTAL= 2.0626

V-mid: N8-C2: 0.197
 N10-C4: 0.217
 N12-C6: 0.208

Bond Order: N8-C2: 1.21
 N10-C4: 1.27
 N12-C6: 1.22
 O17-N8: 2.06
 O18-N8: 1.85
 O19-N10: 2.17
 O20-N10: 1.92
 O21-N12: 2.01
 O22-N12: 1.89

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0

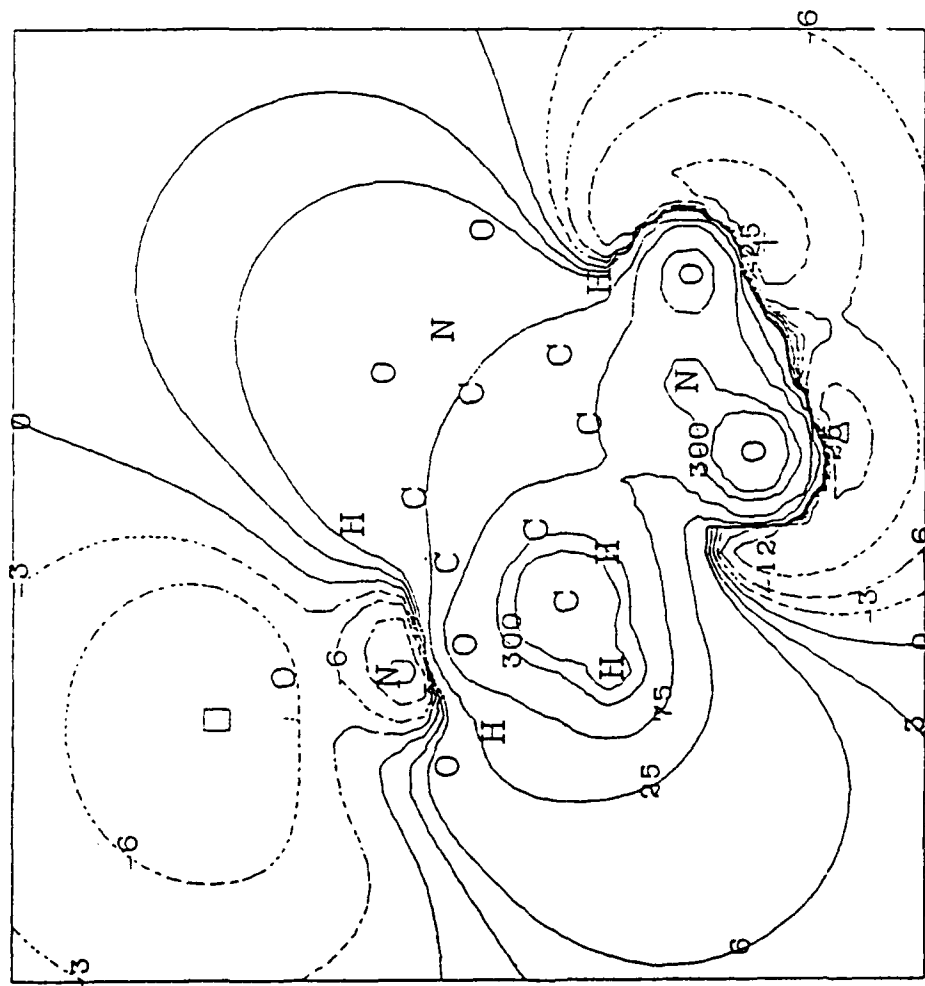


MINIMA

□ -6.746
○ -27.912
△ -38.586
+ -31.256

Figure Z-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0
300.0
600.0



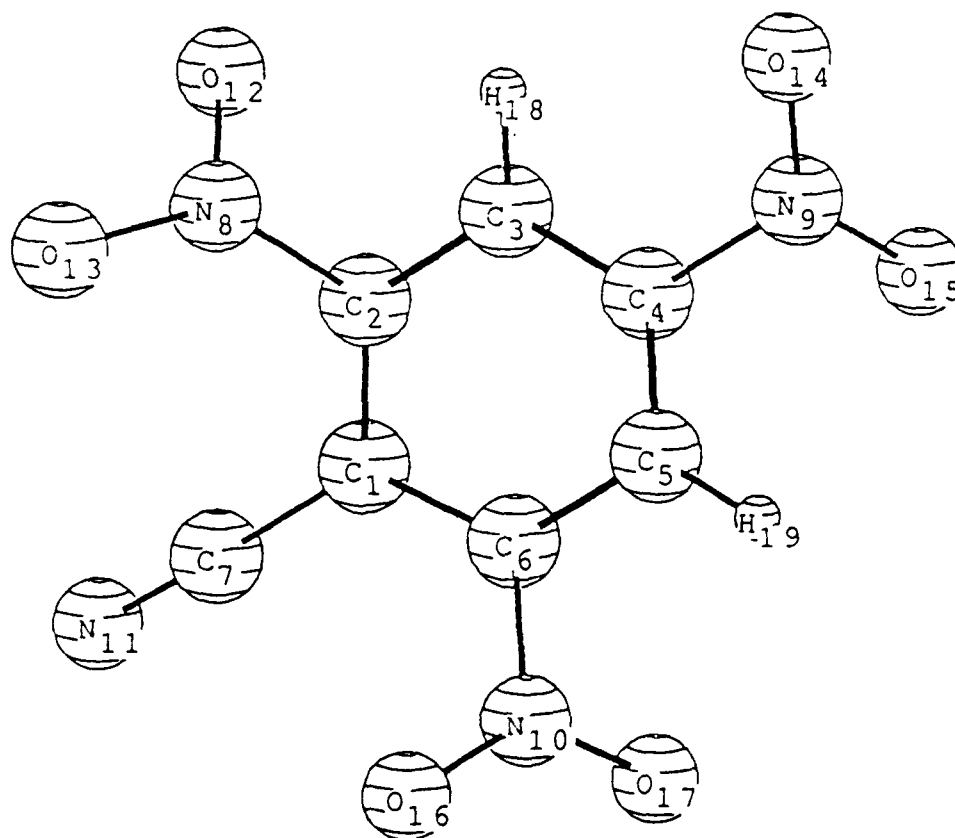
MINIMA
□ -11.502
○ -21.900
△ -35.762
+ -43.806

Figure Z-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzyl alcohol, in the plane 1.75Å above the N12 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX AA
2,4,6-TRINITROBENZONITRILE

The short distances between non-bonded hydrogens and oxygens are H18-O12 (2.39 Å), H18-O14 (2.42 Å), H19-O15 (2.49 Å) and H19-O17 (2.34 Å).

The N8, N9 and N10 nitro groups are rotated out of the mean plane of the benzene ring by approximately 26°, 12° and 16°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.391000 (1)					
3	3	C	2	1.381306 (2)	1	122.868 (19)			
4	4	C	3	1.371322 (3)	2	117.367 (20)	1	-0.952 (36)	0
5	5	C	4	1.358455 (4)	3	123.149 (21)	2	0.610 (37)	0
6	6	C	5	1.384016 (5)	4	117.805 (22)	3	-0.401 (38)	0
7	7	C	1	1.444437 (6)	2	121.382 (23)	3	-174.982 (39)	0
8	8	N	2	1.480487 (7)	3	115.568 (24)	4	177.937 (40)	0
9	9	N	4	1.480034 (8)	3	117.601 (25)	2	-177.192 (41)	0
10	10	N	6	1.485060 (9)	5	116.647 (26)	4	-178.335 (42)	0
11	11	N	7	1.138000 (10)	1	176.811 (27)	2	51.689 (43)	0
12	12	O	8	1.205197 (11)	2	117.195 (28)	1	-154.716 (44)	0
13	13	O	8	1.219426 (12)	2	117.333 (29)	1	26.202 (45)	0
14	14	O	9	1.218041 (13)	4	117.247 (30)	3	12.521 (46)	0
15	15	O	9	1.215971 (14)	4	117.039 (31)	3	-167.466 (47)	0
16	16	O	10	1.208056 (15)	6	117.349 (32)	5	161.878 (48)	0
17	17	O	10	1.214249 (16)	6	116.401 (33)	5	-16.022 (49)	0
18	18	H	3	1.000000 (17)	4	122.543 (34)	5	179.414 (50)	0
19	19	H	5	1.000000 (18)	4	123.385 (35)	3	-172.430 (51)	0

STOICHIOMETRY C7H2N4O6

SCF DONE: E(RHF) = -928.874944710

EIGENVALUES — -0.38909 -0.38680 -0.33299 -0.32951 -0.32956 0.08269

Estimated ionization potential: 8.95 ev

TOTAL ATOMIC CHARGES.

	1	Net Charge
1 C	5.959718	0.040
2 C	5.884293	0.116
3 C	6.047682	-0.048
4 C	5.889990	0.110
5 C	6.050620	-0.051
6 C	5.884619	0.115
7 C	5.896436	0.104
8 N	6.818527	0.181
9 N	6.821234	0.179
10 N	6.815834	0.184
11 N	7.138529	-0.139
12 O	8.184625	-0.185
13 O	8.179035	-0.179
14 O	8.187497	-0.187
15 O	8.184231	-0.184
16 O	8.175735	-0.176
17 O	8.187217	-0.187
18 H	0.847320	0.153
19 H	0.846857	0.153

DIPOLE MOMENT (DEBYE): X= 2.0748 Y=-0.0299 Z= 1.1260 TOTAL= 2.3609

Bond Order: C2-N8: 1.21

V-mid: C2-N8: 0.213

C4-N9: 1.21

C4-N9: 0.207

C6-N10: 1.20

C6-N10: 0.213

N8-O12: 2.01

N8-O13: 1.94

N9-O14: 1.95

N9-O15: 1.96

N10-O16: 2.00

N10-O17: 1.97

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0
300.0
600.0

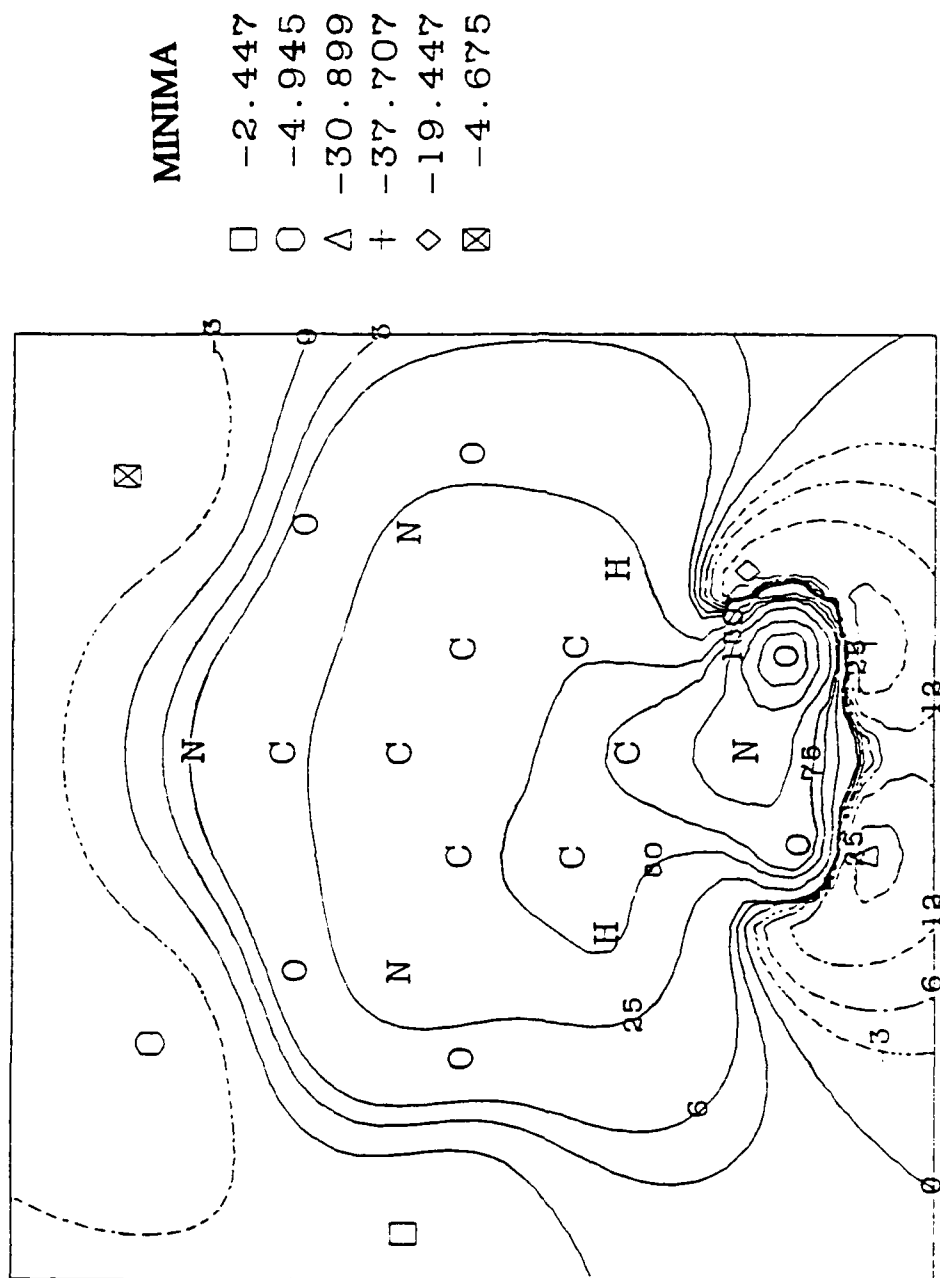
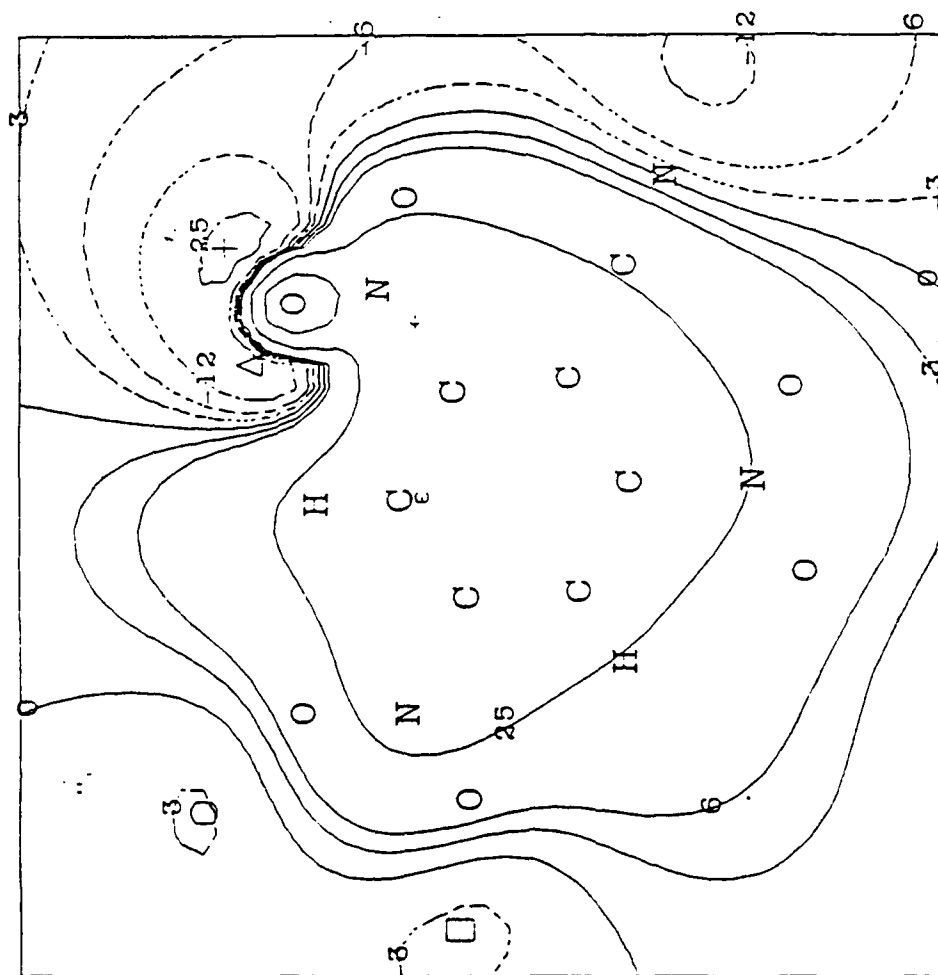


Figure AA-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
75.0



MINIMA

□ -3.432
○ -3.144
△ -21.542
+ -30.767

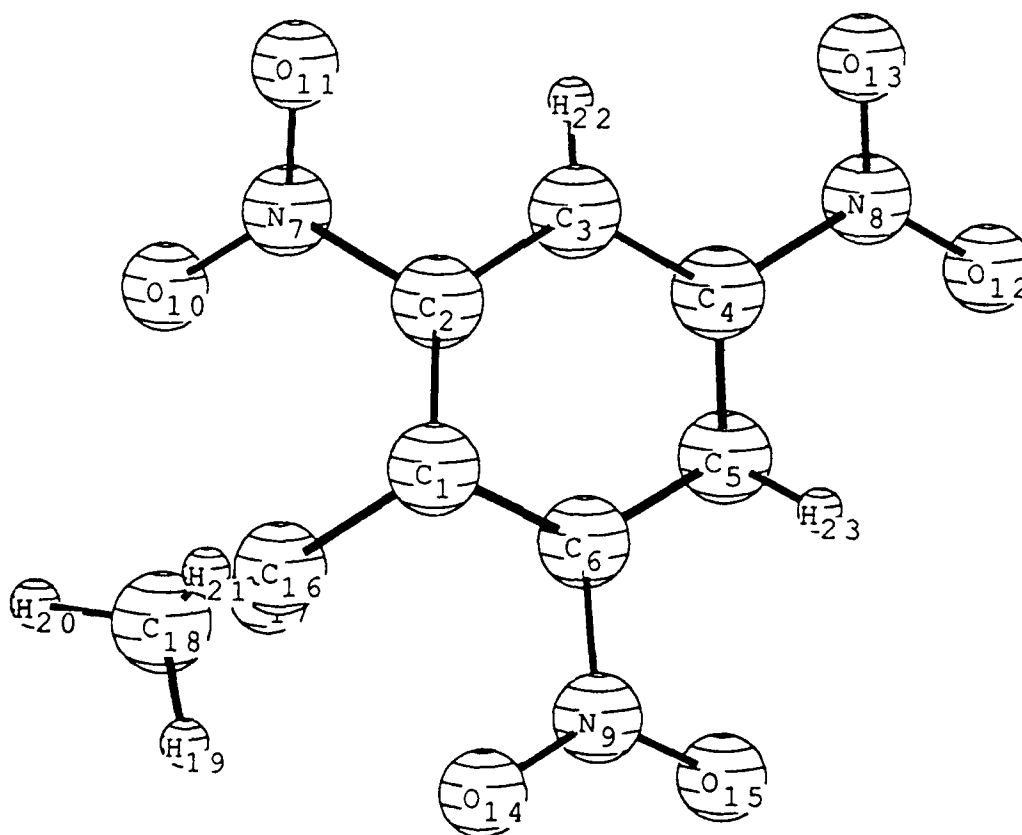
MAXIMA

ε +44.554
+ +50.201

Figure AA-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitrobenzonitrile, in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX BB
2,4,6-TRINITROACETOPHENONE

The short distances between non-bonded hydrogens and oxygens are H19-O14 (2.50 Å), H22-O11 (2.34 Å), H22-O13 (2.47 Å), H23-O12 (2.48 Å), and H23-O15 (2.40 Å). Nitro groups N7, N8 and N9 are rotated out of the plane by approximately 4°, 18° and 20°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.392000 (1)					
3	3	C	2	1.376431 (2)	1	124.036 (23)			
4	4	C	3	1.378529 (3)	2	117.369 (24)	1	2.057 (44)	0
5	5	C	4	1.369033 (4)	3	122.420 (25)	2	-1.476 (45)	0
6	6	C	5	1.374375 (5)	4	117.646 (26)	3	-0.430 (46)	0
7	7	N	2	1.482075 (6)	3	116.031 (27)	4	-177.045 (47)	0
8	8	N	4	1.467600 (7)	3	118.482 (28)	2	177.754 (48)	0
9	9	N	6	1.476630 (8)	5	116.075 (29)	4	-178.568 (49)	0
10	10	O	7	1.217664 (9)	2	117.865 (30)	3	175.152 (50)	0
11	11	O	7	1.211071 (10)	2	117.785 (31)	3	-4.138 (51)	0
12	12	O	8	1.223031 (11)	4	117.572 (32)	3	-162.894 (52)	0
13	13	O	8	1.215320 (12)	4	117.940 (33)	3	17.721 (53)	0
14	14	O	9	1.221059 (13)	6	117.270 (34)	5	160.112 (54)	0
15	15	O	9	1.220414 (14)	6	118.112 (35)	5	-20.335 (55)	0
16	16	C	1	1.536863 (15)	2	123.236 (36)	3	-176.449 (56)	0
17	17	O	16	1.202061 (16)	1	117.552 (37)	2	91.705 (57)	0
18	18	C	16	1.488976 (17)	1	117.877 (38)	2	-88.268 (58)	0
19	19	H	18	0.945258 (18)	16	105.483 (39)	1	-105.217 (59)	0
20	20	H	18	0.984491 (19)	16	108.722 (40)	1	136.333 (60)	0
21	21	H	18	0.880823 (20)	16	114.232 (41)	1	6.666 (61)	0
22	22	H	3	0.932775 (21)	2	120.931 (42)	1	179.643 (62)	0
23	23	H	5	0.905621 (22)	4	122.221 (43)	3	-177.399 (63)	0

STOICHIOMETRY C8H5N3O7

SCF DONE: E(RHF) = -988.555699827 A.U. AFTER 41 CYCLES

EIGENVALUES -- -0.38134 -0.37535 -0.32540 -0.32376 -0.31771 0.10850

Estimated ionization potential: 8.66 eV

TOTAL ATOMIC CHARGES.

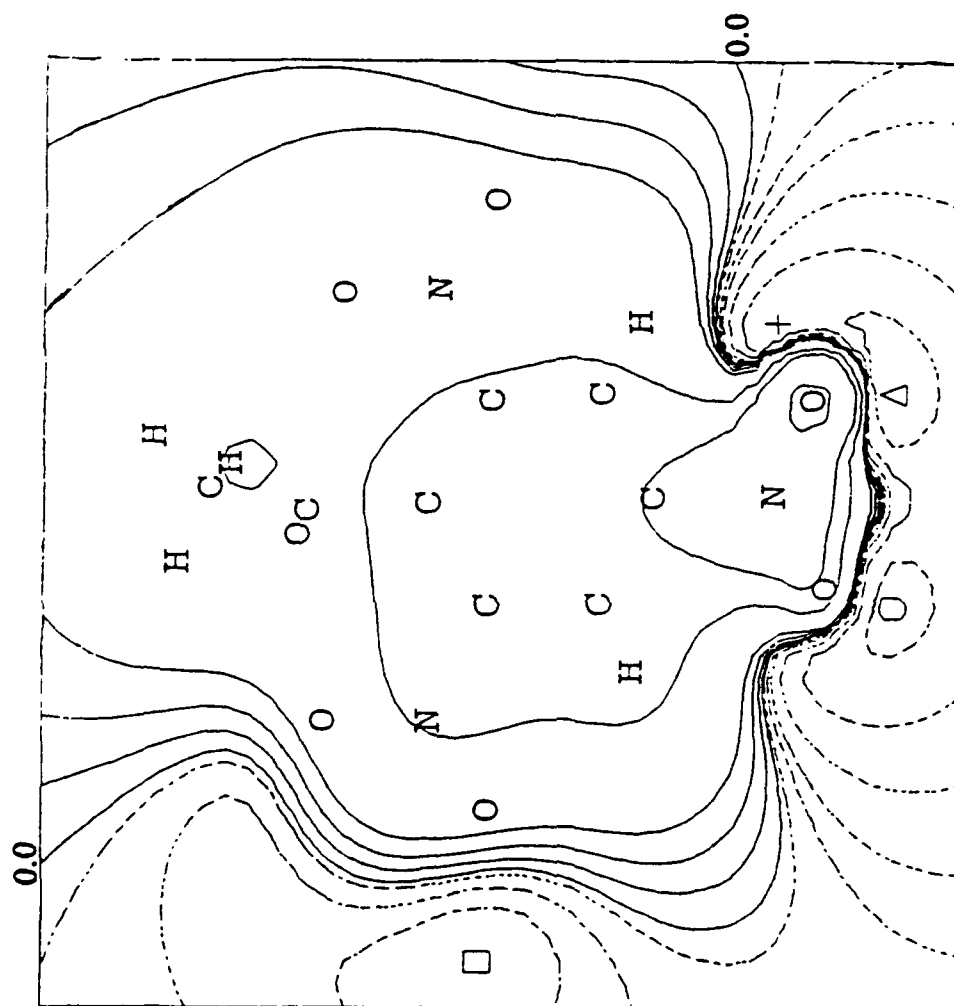
		1	Net Charge
1	C	5.977507	0.022
2	C	5.899033	0.101
3	C	6.067820	-0.068
4	C	5.882452	0.118
5	C	6.077950	-0.078
6	C	5.894200	0.106
7	N	6.821736	0.178
8	N	6.827279	0.173
9	N	6.827353	0.173
10	O	8.196196	-0.196
11	O	8.185658	-0.186
12	O	8.189231	-0.189
13	O	8.187950	-0.188
14	O	8.198360	-0.198
15	O	8.180660	-0.181
16	C	5.715981	0.284
17	O	8.212960	-0.213
18	C	6.369110	-0.369
19	H	0.855457	0.145
20	H	0.865263	0.135
21	H	0.874293	0.126
22	H	0.846495	0.154
23	H	0.847056	0.153

DIPOLE MOMENT (DEBYE): X=-0.2659 Y=-1.8122 Z=-0.0756 TOTAL= 1.8332

V-mid: N7-C2: 0.199
N8-C4: 0.210
N9-C6: 0.200

Bond Order: N7-C2: 1.21
N8-C4: 1.25
N9-C6: 1.22
O10-N7: 1.95
O11-N7: 1.98
O12-N8: 1.92
O13-N8: 1.96
O14-N9: 1.93
O15-N9: 1.94

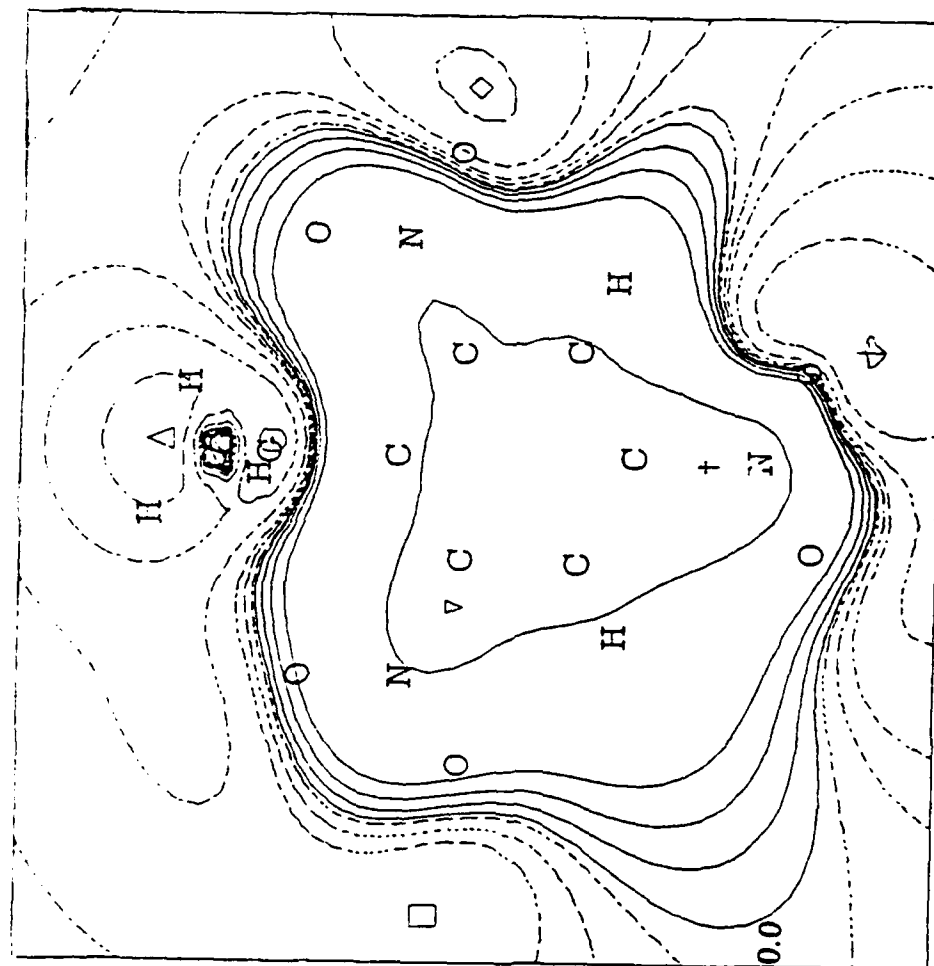
0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 62.751
 313.754
 0.000



MINIMA
 □ -4.311
 ○ -32.756
 △ -41.190
 + -23.946

Figure BB-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

0.000
 -25.100
 -12.550
 -6.275
 -3.138
 -1.883
 -0.628
 1.255
 3.138
 6.275
 31.375
 0.000



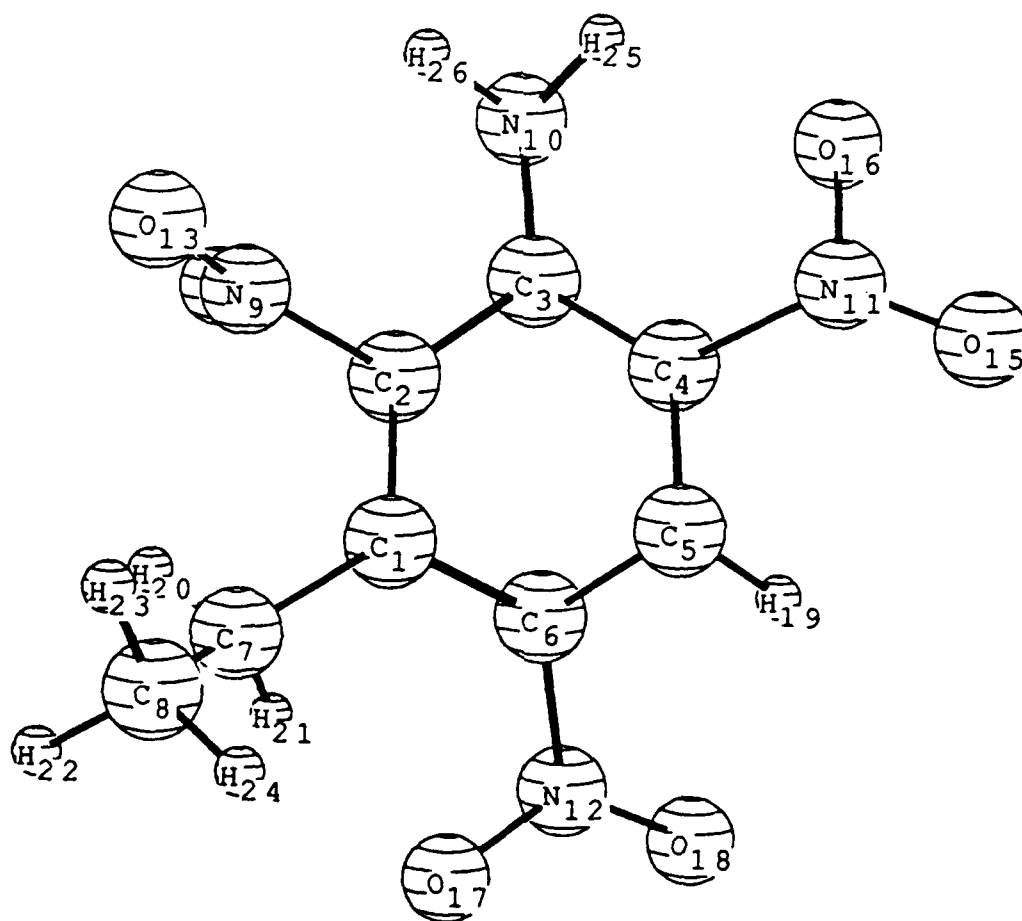
MINIMA	
□	-5.196
○	-25.653
△	-39.577
+	-25.985
◇	-13.862
MAXIMA	
▽	36.057
+	45.915

Figure BB-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitroacetophenone in the plane 1.75Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX CC
3-AMINO-2,4,6-TRINITROETHYLBENZENE

The short distances between non-bonded hydrogens and oxygens are H19-O18 (2.22 Å), H19-O15 (2.51 Å) and H25-O16 (2.19 Å).

The N11 and N12 nitro groups are rotated out of the mean plane of the benzene ring by approximately 27° and 16°. The N9 nitro group is essentially perpendicular to the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.386000(1)				
3	3	C	2	1.422212(2)	1	126.283(26)		
4	4	C	3	1.391275(3)	2	114.113(27)	1	-2.941(50)
5	5	C	4	1.389812(4)	3	123.198(28)	2	2.752(51)
6	6	C	5	1.384322(5)	4	119.091(29)	3	0.643(52)
7	7	C	1	1.501938(6)	2	122.276(30)	3	178.570(53)
8	8	C	7	1.520060(7)	1	112.660(31)	2	-93.121(54)
9	9	N	2	1.459146(8)	3	114.752(32)	4	177.008(55)
10	10	N	3	1.346982(9)	4	125.719(33)	5	-176.846(56)
11	11	N	4	1.561775(10)	5	114.391(34)	6	-178.704(57)
12	12	N	6	1.481676(11)	5	114.336(35)	4	174.042(58)
13	13	O	9	1.200006(12)	2	118.610(36)	1	92.920(59)
14	14	O	9	1.201423(13)	2	117.837(37)	1	-89.338(60)
15	15	O	11	1.177512(14)	4	114.655(38)	5	-27.223(61)
16	16	O	11	1.213044(15)	4	113.581(39)	5	162.132(62)
17	17	O	12	1.235447(16)	6	118.156(40)	5	165.583(63)
18	18	O	12	1.209812(17)	6	118.461(41)	5	-16.250(64)
19	19	H	5	1.003240(18)	4	126.191(42)	3	173.591(65)
20	20	H	7	1.000000(19)	1	109.900(43)	2	28.400(66)
21	21	H	7	1.000000(20)	1	110.300(44)	2	144.100(67)
22	22	H	8	1.000000(21)	7	108.900(45)	1	176.600(68)
23	23	H	8	1.000000(22)	7	110.700(46)	1	57.100(69)
24	24	H	8	1.000000(23)	7	110.300(47)	1	-64.000(70)
25	25	H	10	0.953232(24)	3	130.456(48)	4	-2.515(71)
26	26	H	10	0.996377(25)	3	127.439(49)	4	-159.940(72)

STOICHIOMETRY C8H8N4O6

CF DONE: E(RHF) = -970.119859474

Alpha eigenvalues — -0.30137 0.14867 0.15733 0.20240 0.22068

Estimated ionization potential: 8.20 ev

Total atomic charges:

1
 1 C 0.069481
 2 C 0.061105
 3 C 0.190756
 4 C 0.051414
 5 C -0.044100
 6 C 0.061606
 7 C -0.153866
 8 C -0.250476
 9 N 0.175508
 10 N -0.460750
 11 N 0.207898
 12 N 0.168658
 13 O -0.208019
 14 O -0.198304
 15 O -0.187484
 16 O -0.221248
 17 O -0.207781
 18 O -0.198601
 19 H 0.141595
 20 H 0.095855
 21 H 0.118446
 22 H 0.098428
 23 H 0.092596
 24 H 0.098893
 25 H 0.264199
 26 H 0.234191

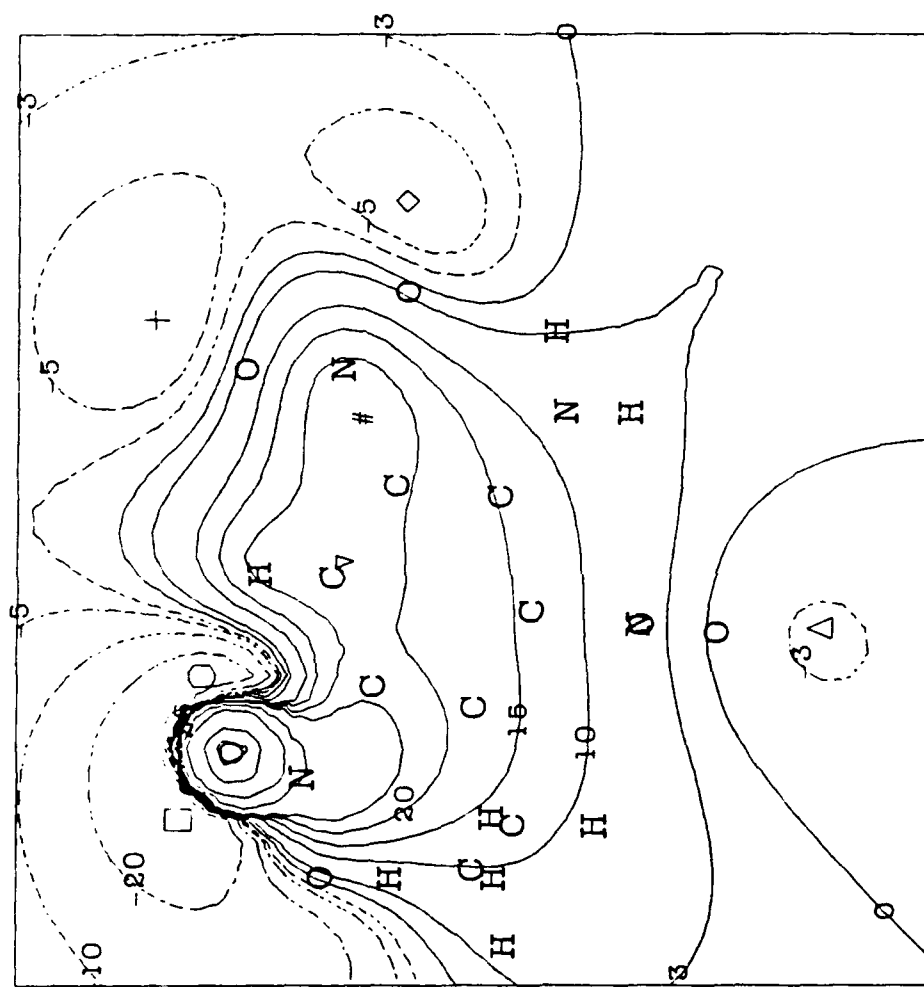
Dipole moment (Debye):

X= 0.7115 Y= 2.0184 Z= 0.6089 Tot= 2.2250

Bond Order: C2-N9: 1.27
 C4-N11: 1.03
 C6-N12: 1.21
 N9-O13: 2.04
 N9-O14: 2.03
 N11-O15: 2.15
 N11-O16: 1.97
 N12-O17: 1.87
 N12-O18: 1.99

V-mid: C2-N9: 0.172
 C4-N11: 0.176
 C6-N12: 0.165

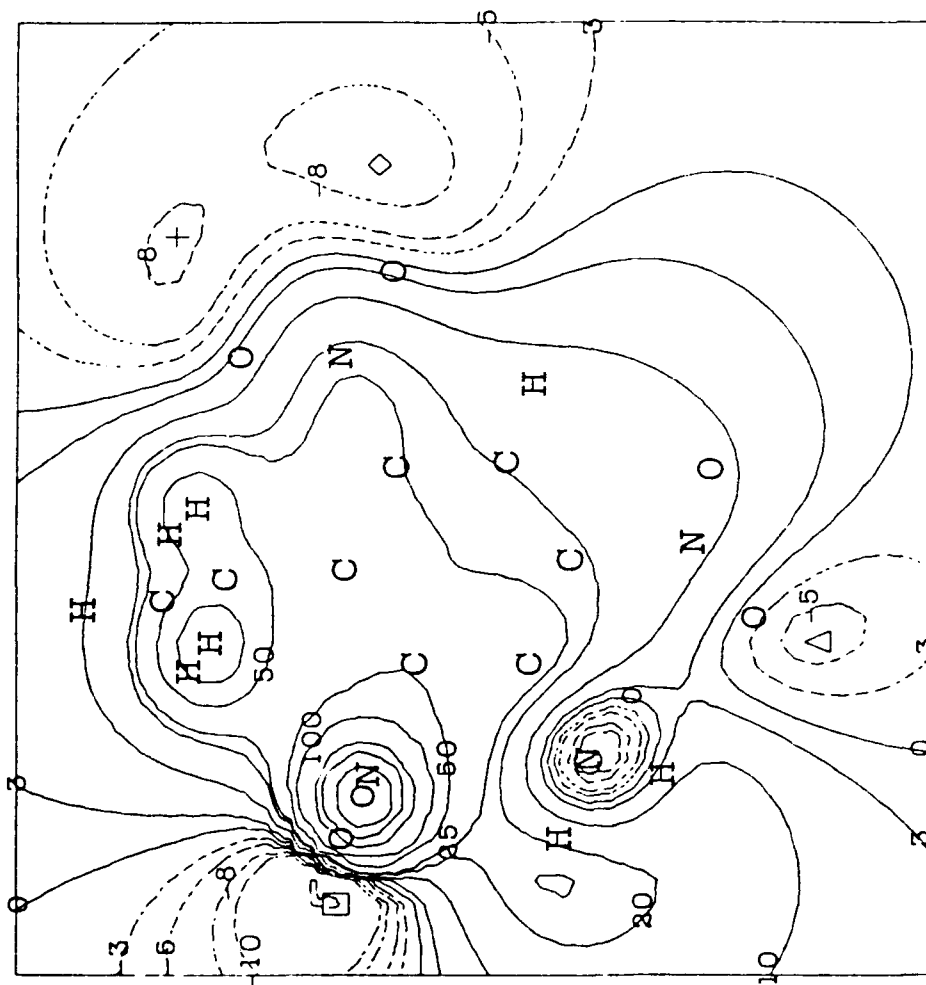
-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
15.0
20.0
25.0
50.0
100.0
300.0
500.0



MINIMA		MAXIMA	
□	-48.1	▽	+23.4
○	-31.9	#	+24.0
△	-3.2		
+	-7.5		
◇	-7.1		

Figure CC-1. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N11 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-8.0
-5.0
-3.0
0.0
3.0
10.0
20.0
25.0
50.0
100.0
300.0
500.0
1000.0



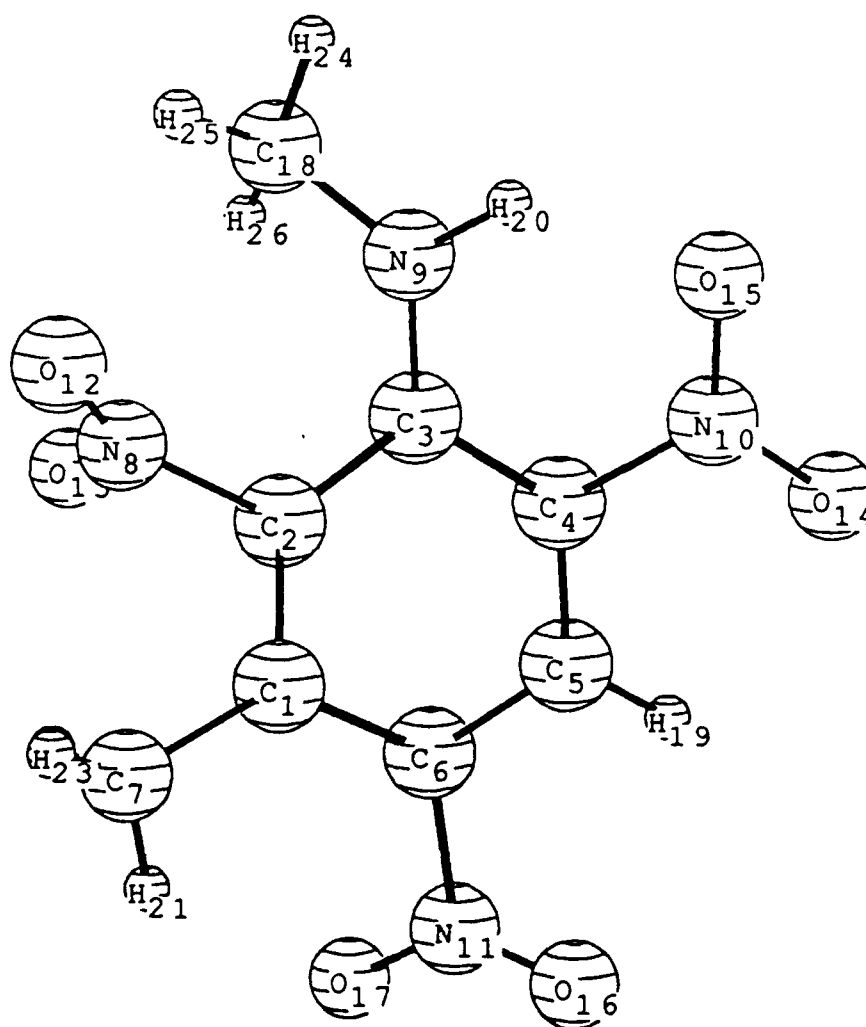
MINIMA
□ -20.6
○ -12.9
△ -5.7
+ -8.3
◇ -9.5

Figure CC-2. Calculated electrostatic potential, in kcal/mole, of 3-amino-2,4,6-trinitroethylbenzene, in the plane 1.75Å above the N12 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX DD
3-(METHYLAMINO)-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H20-O15 (1.86 Å), H19-O14 (2.30 Å), H21-O17 (2.12 Å), H19-O16 (2.39 Å) and H25-O12 (2.26 Å).

The N10 nitro group is rotated by only a few degrees, while the N8 and N11 nitro groups are rotated by about 70° and 28°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C	1	1.387000(1)				
3	3	C	2	1.423402(2)	1	127.514(26)		
4	4	C	3	1.414310(3)	2	112.226(27)	1	2.928(50) 0
5	5	C	4	1.361095(4)	3	123.213(28)	2	-0.621(51) 0
6	6	C	5	1.369364(5)	4	119.928(29)	3	1.216(52) 0
7	7	C	1	1.504085(6)	2	120.357(30)	3	170.734(53) 0
8	8	N	2	1.499699(7)	3	117.269(31)	4	172.945(54) 0
9	9	N	3	1.349787(8)	4	122.693(32)	5	-178.451(55) 0
10	10	N	4	1.457821(9)	3	121.264(33)	2	-178.502(56) 0
11	11	N	6	1.488813(10)	1	122.291(34)	2	-177.188(57) 0
12	12	O	8	1.220013(11)	2	119.017(35)	3	-70.735(58) 0
13	13	O	8	1.226737(12)	2	115.633(36)	3	110.924(59) 0
14	14	O	10	1.197185(13)	4	118.962(37)	3	-174.738(60) 0
15	15	O	10	1.216527(14)	4	120.361(38)	3	3.579(61) 0
16	16	O	11	1.194307(15)	6	118.935(39)	1	-150.067(62) 0
17	17	O	11	1.235850(16)	6	116.752(40)	1	27.060(63) 0
18	18	C	9	1.457548(17)	3	130.576(41)	4	167.728(64) 0
19	19	H	5	0.960345(18)	4	120.147(42)	3	-178.965(65) 0
20	20	H	9	0.960046(19)	3	114.694(43)	2	170.062(66) 0
21	21	H	7	0.959826(20)	1	109.497(44)	2	-179.929(67) 0
22	22	H	7	0.959953(21)	1	109.504(45)	2	59.960(68) 0
23	23	H	7	0.959828(22)	1	109.307(46)	2	-59.986(69) 0
24	24	H	18	0.960065(23)	9	109.439(47)	3	179.924(70) 0
25	25	H	18	0.960356(24)	9	109.528(48)	3	59.925(71) 0
26	26	H	18	0.959395(25)	9	109.456(49)	3	-60.081(72) 0

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.075763639

Alpha eigenvalues — -0.29218 0.13740 0.15765 0.19042 0.22757

Estimated ionization potential: 7.95 ev

Total atomic charges:

1

1	C	0.085271
2	C	0.053151
3	C	0.188005
4	C	0.054806
5	C	-0.054473
6	C	0.063076
7	C	-0.322866
8	N	0.163997
9	N	-0.368273
10	N	0.182207
11	N	0.176478
12	O	-0.199149
13	O	-0.195273
14	O	-0.189983
15	O	-0.232787
16	O	-0.193338
17	O	-0.214760
18	C	-0.198122
19	H	0.147237
20	H	0.271281
21	H	0.143786
22	H	0.133790
23	H	0.124860
24	H	0.127866
25	H	0.130127
26	H	0.122087

Dipole moment (Debye):

X= -2.7288 Y= -0.7028 Z= -0.0840 Tot= 2.8191

Bond Order: C2-N8: 1.17	V-mid: C2-N8: 0.153
C4-N10: 1.27	C4-N10: 0.172
C6-N11: 1.19	C6-N11: 0.170
N8-O12: 1.94	
N8-O13: 1.89	
N10-O14: 2.05	
N10-O15: 1.96	
N11-O16: 2.07	
N11-O17: 1.86	

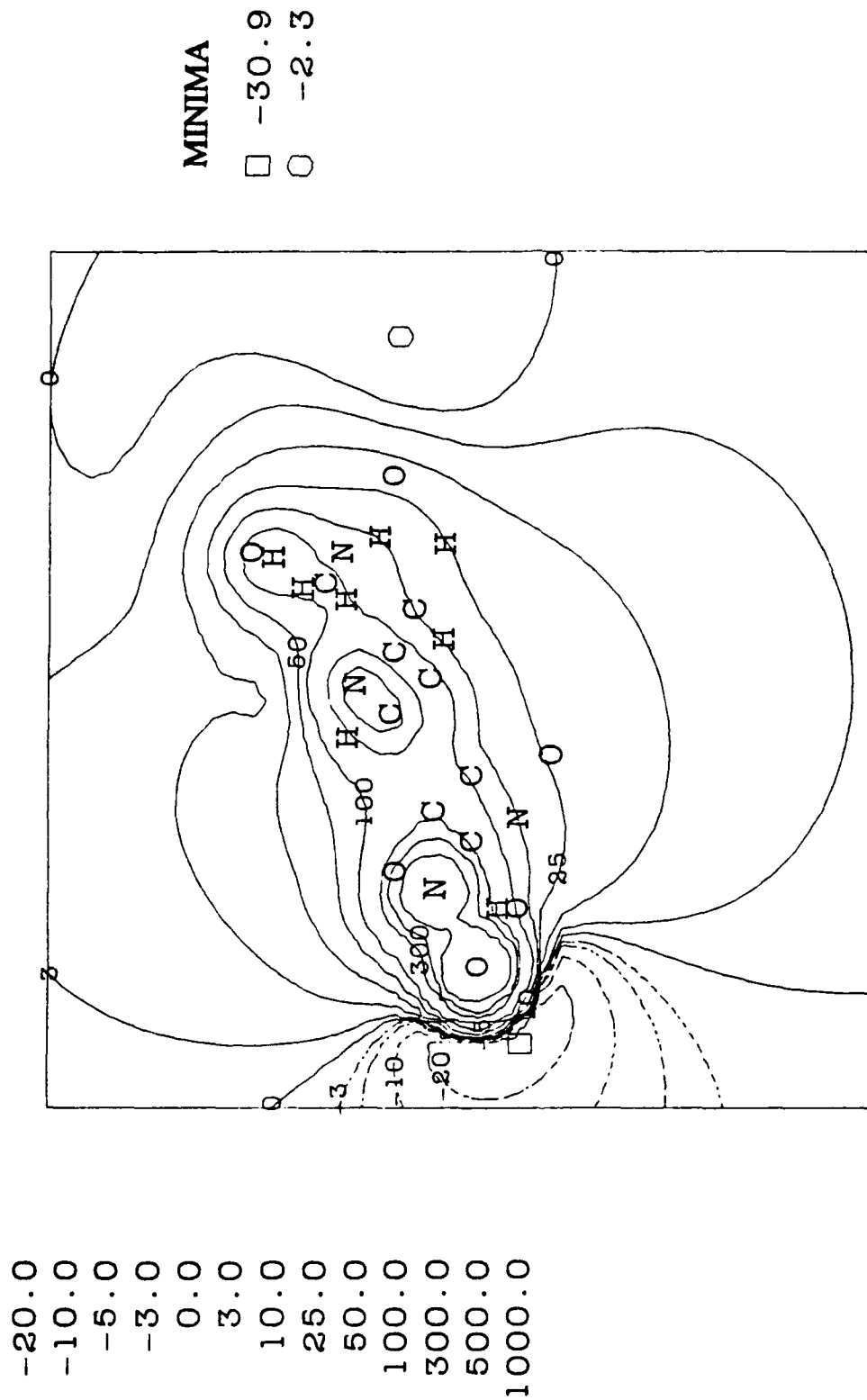
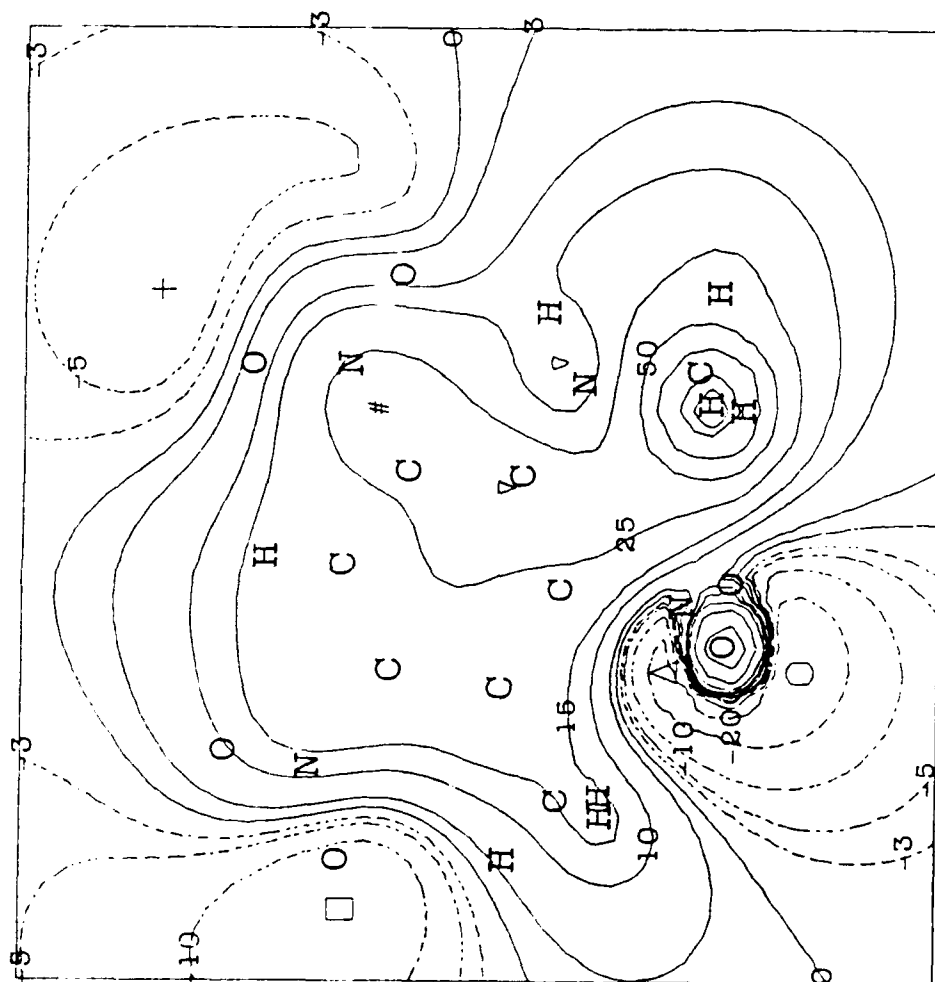


Figure DD-1. Calculated electrostatic potential, in kcal/mole, of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75 Å above the N8 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
15.0
25.0
50.0
100.0
300.0
500.0



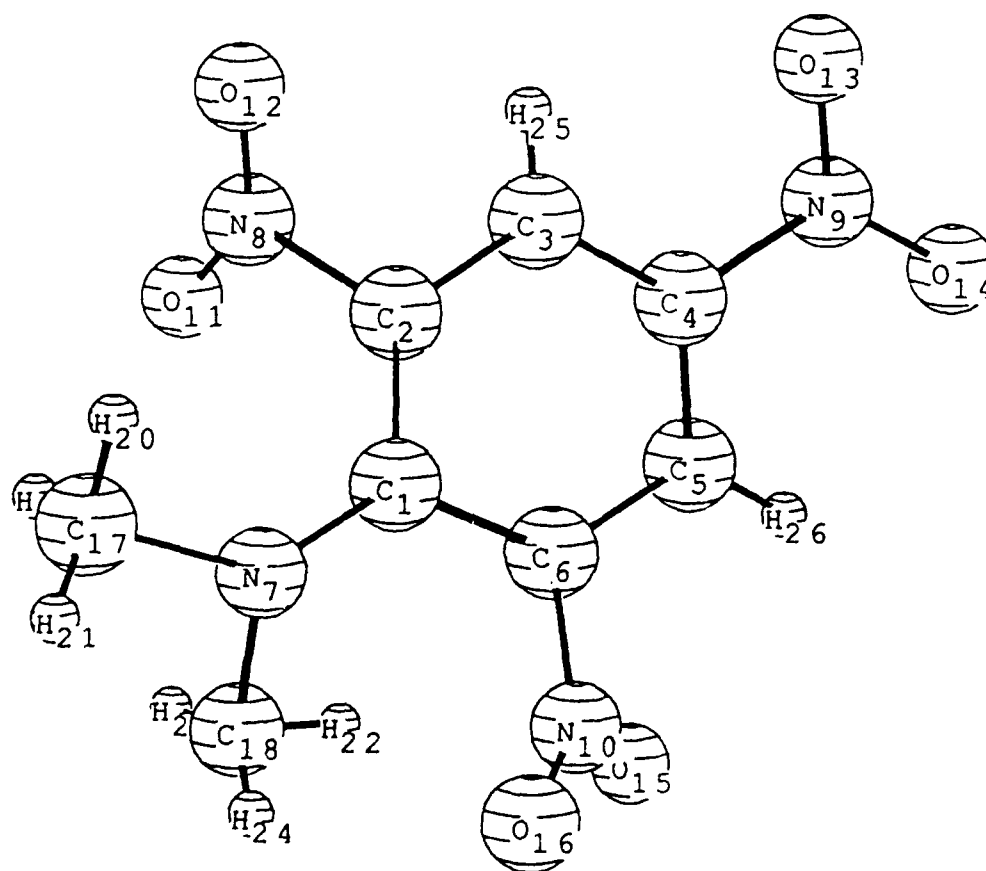
MINIMA	
□	-19.1
○	-33.2
△	-28.5
+	-7.5
MAXIMA	
▽	+32.8
#	+29.7

Figure DD-2. Calculated electrostatic potential, in kcal/mole, of 3-(methylamino)-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX EE
N,N-DIMETHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H19-O11 (2.45 Å), H25-O12 (2.44 Å), H25-O13 (2.47 Å) and H26-O14 (2.46 Å).

The N8 and N10 nitro groups are rotated out of the mean plane of the benzene ring by about 40° and 60°, respectively an the N9 nitro group is only rotated by about 12°.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.423000 (1)					
3	3	C	2	1.374045 (2)	1	123.619 (26)			
4	4	C	3	1.370644 (3)	2	119.225 (27)	1	5.404 (50)	0
5	5	C	4	1.376151 (4)	3	120.869 (28)	2	-0.276 (51)	0
6	6	C	5	1.372077 (5)	4	118.960 (29)	3	-3.120 (52)	0
7	7	N	1	1.349478 (6)	2	123.521 (30)	3	173.695 (53)	0
8	8	N	2	1.464762 (7)	3	114.848 (31)	4	-167.543 (54)	0
9	9	N	4	1.463054 (8)	3	119.319 (32)	2	-179.969 (55)	0
10	10	N	6	1.472506 (9)	5	114.518 (33)	4	-170.478 (56)	0
11	11	O	8	1.221450 (10)	2	117.933 (34)	3	137.037 (57)	0
12	12	O	8	1.223656 (11)	2	117.859 (35)	3	-38.607 (58)	0
13	13	O	9	1.218935 (12)	4	118.151 (36)	3	12.204 (59)	0
14	14	O	9	1.216440 (13)	4	117.945 (37)	3	-167.562 (60)	0
15	15	O	10	1.217251 (14)	6	117.309 (38)	5	-61.719 (61)	0
16	16	O	10	1.218075 (15)	6	117.586 (39)	5	116.650 (62)	0
17	17	C	7	1.455934 (16)	1	122.585 (40)	2	-34.804 (63)	0
18	18	C	7	1.461052 (17)	1	123.541 (41)	2	146.862 (64)	0
19	19	H	17	0.958692 (18)	7	110.528 (42)	1	111.392 (65)	0
20	20	H	17	0.990708 (19)	7	112.964 (43)	1	-8.518 (66)	0
21	21	H	17	0.959269 (20)	7	108.882 (44)	1	-128.428 (67)	0
22	22	H	18	1.030678 (21)	7	111.441 (45)	1	-15.326 (68)	0
23	23	H	18	0.946545 (22)	7	108.101 (46)	1	-134.306 (69)	0
24	24	H	18	0.945969 (23)	7	110.604 (47)	1	102.403 (70)	0
25	25	H	3	0.919951 (24)	2	119.186 (48)	1	179.212 (71)	0
26	26	H	5	0.901762 (25)	4	120.486 (49)	3	179.569 (72)	0

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.023626858

EIGENVALUES — -0.29462 0.13090 0.14078 0.18718 0.22142

Estimated ionization potential: 8.03 eV

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.816149	0.184
2	C	5.923220	0.077
3	C	6.066100	-0.066
4	C	5.905775	0.094
5	C	6.071256	-0.071
6	C	5.919412	0.081
7	N	7.257770	-0.258
8	N	6.834545	0.165
9	N	6.827066	0.173
10	N	6.830101	0.170
11	O	8.197192	-0.197
12	O	8.194999	-0.195
13	O	8.198365	-0.199
14	O	8.198555	-0.199
15	O	8.192531	-0.193
16	O	8.195733	-0.196
17	C	6.187701	-0.188
18	C	6.185064	-0.185
19	H	0.874728	0.125
20	H	0.887417	0.113
21	H	0.880816	0.119
22	H	0.889906	0.110
23	H	0.877204	0.123
24	H	0.875449	0.125
25	H	0.854898	0.145
26	H	0.858047	0.142

DIPOLE MOMENT (DEBYE): X=-2.9260 Y=-0.4301 Z=-2.0966 TOTAL= 3.6252

Bond Order: C2-N8: 1.25

V-mid: C2-N8: 0.175

C4-N9: 1.26

C4-N9: 0.193

C6-N10: 1.23

C6-N10: 0.180

N8-O11: 1.93

N8-O12: 1.92

N9-O13: 1.94

N9-O14: 1.96

N10-O15: 1.95

N10-O16: 1.95

-15.0
 -10.0
 -6.0
 -3.0
 0.0
 3.0
 6.0
 12.0
 18.0
 25.0
 30.0
 35.0
 50.0
 75.0
 160.0
 300.0
 600.0
 1000.0

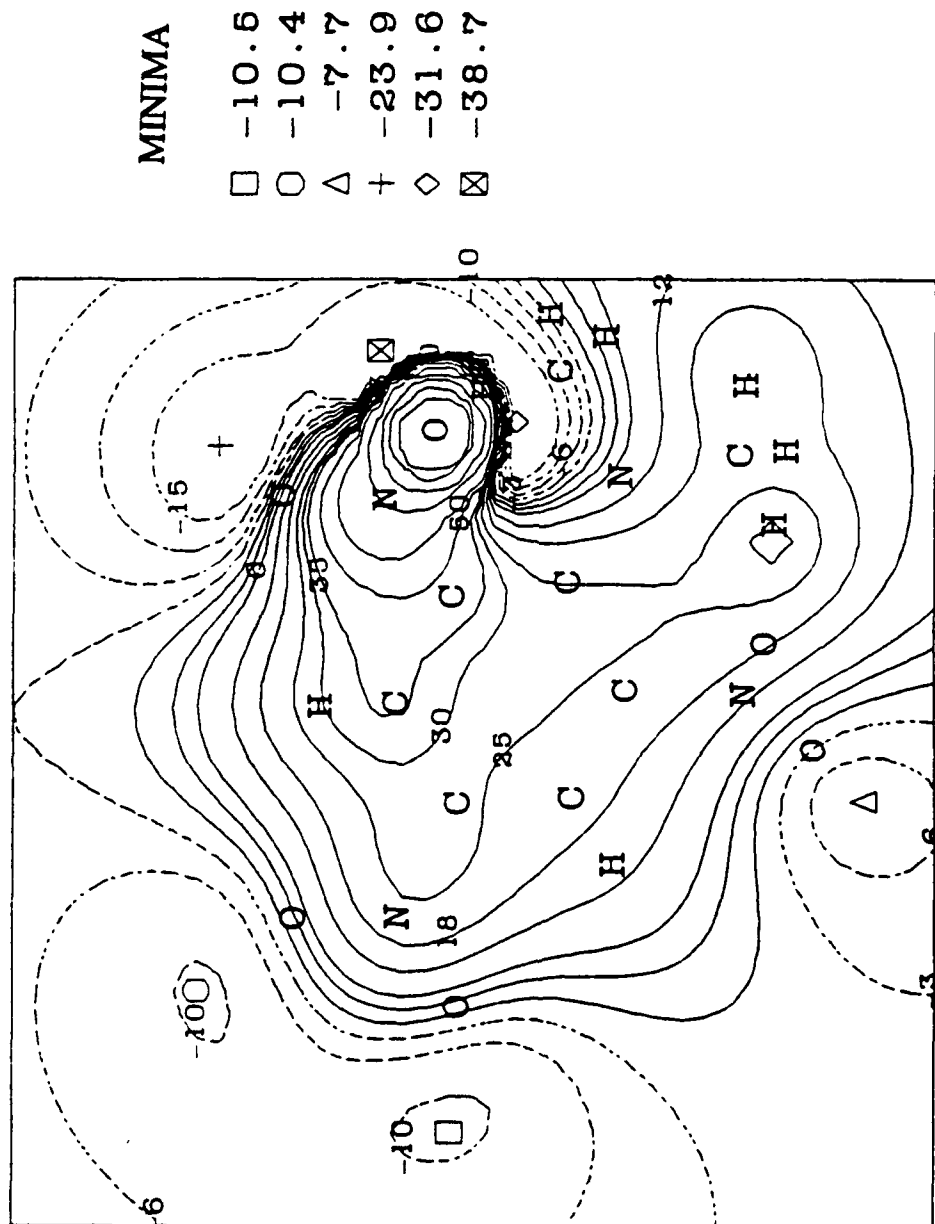


Figure EE-1. Calculated electrostatic potential, in kcal/mole, of N,N-dimethylpicramide, in the plane 1.75 Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
18.0
25.0
35.0
50.0
75.0
150.0
300.0
600.0
1000.0

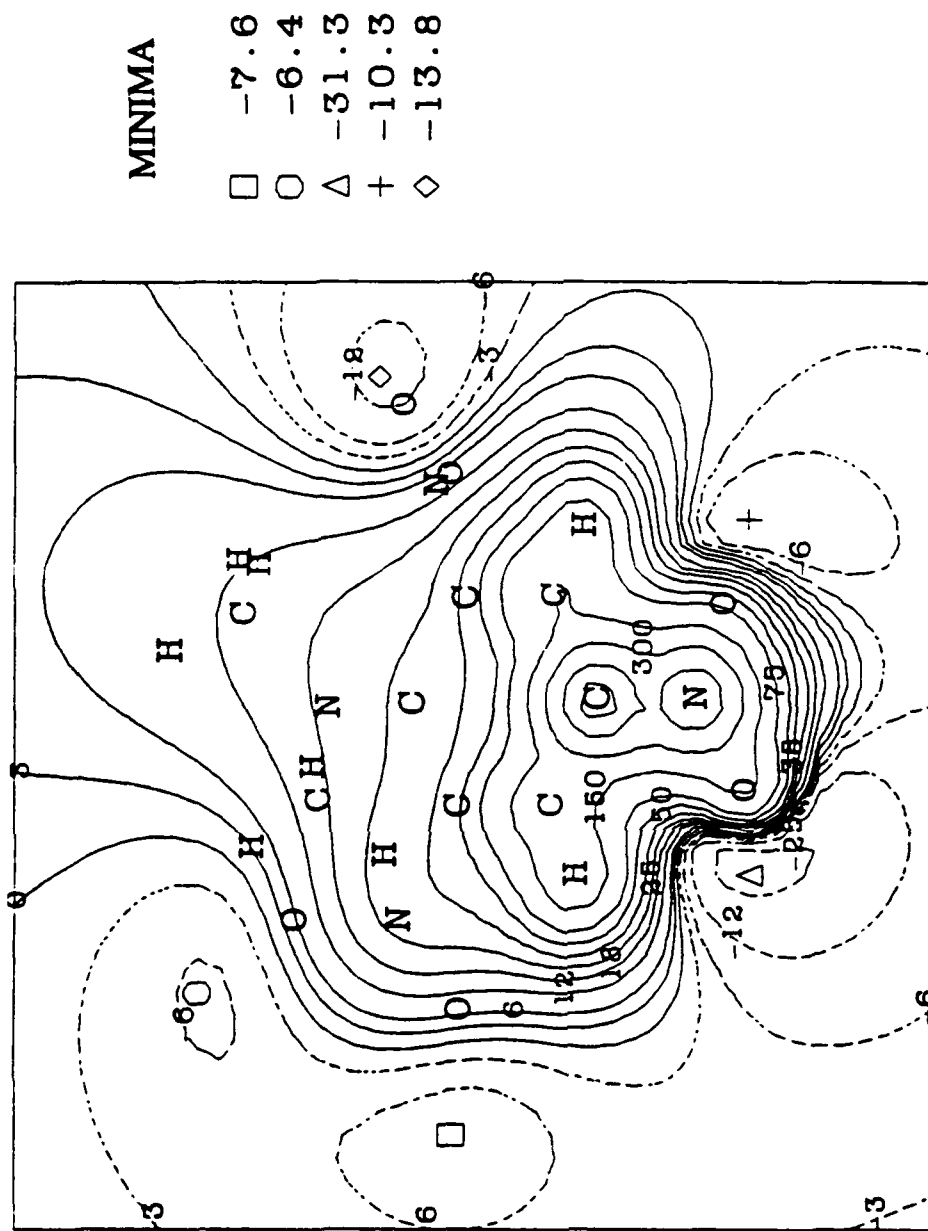
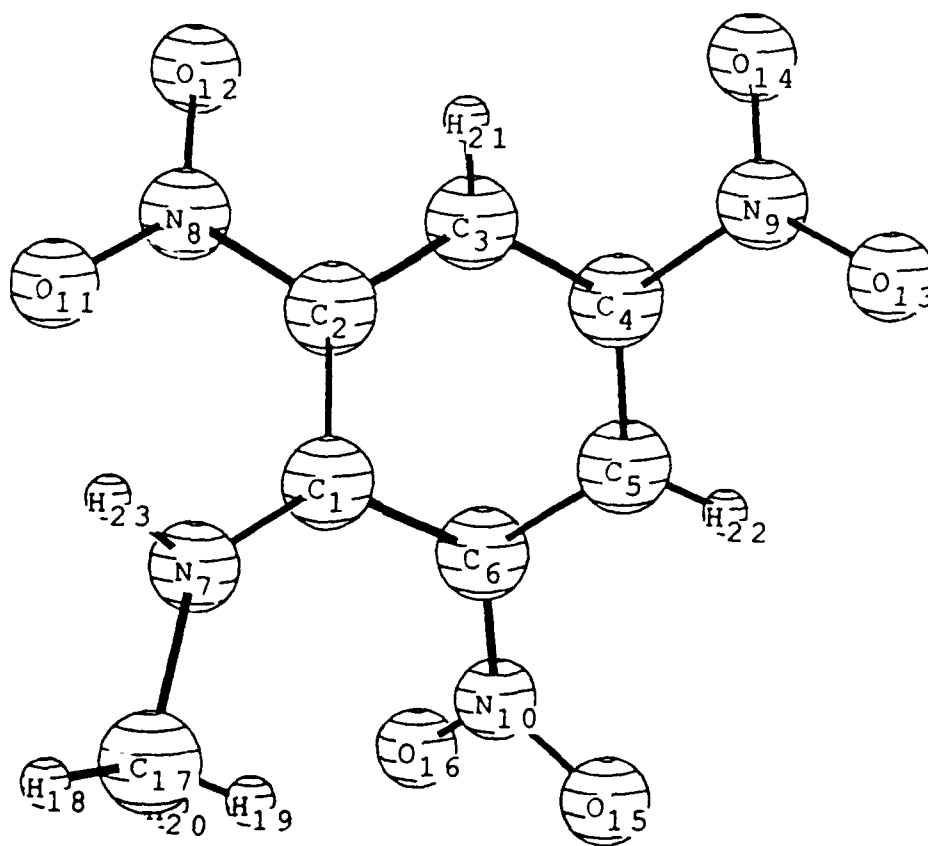


Figure EE-2. Calculated electrostatic potential, in kcal/mole, of N,N-dimethylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX FF N-METHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H21-O12 (2.31 Å), H23-O11 (1.84 Å), H22-O13 (2.40 Å), H21-O14 (2.44 Å) and H20-O16 (2.38 Å).

The N10 nitro group is rotated out of the mean plane of the benzene ring by approximately 50°, while the N8 and N9 nitro groups are only rotated by about 6° and 9°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA
								J
1	1	C						
2	2	C	1	1.436000 (1)				
3	3	C	2	1.365763 (2)	1	122.514 (23)		
4	4	C	3	1.370295 (3)	2	120.392 (24)	1	0.531 (44) 0
5	5	C	4	1.373754 (4)	3	120.663 (25)	2	5.753 (45) 0
6	6	C	5	1.377130 (5)	4	118.833 (26)	3	-3.536 (46) 0
7	7	N	1	1.333529 (6)	2	122.351 (27)	3	168.686 (47) 0
8	8	N	2	1.454798 (7)	3	115.942 (28)	4	-179.970 (48) 0
9	9	N	4	1.456627 (8)	5	120.414 (29)	6	179.874 (49) 0
10	10	N	6	1.458624 (9)	5	114.713 (30)	4	169.974 (50) 0
11	11	O	8	1.230412 (10)	2	119.737 (31)	1	5.834 (51) 0
12	12	O	8	1.216932 (11)	2	118.158 (32)	1	-173.058 (52) 0
13	13	O	9	1.228128 (12)	4	117.256 (33)	5	-9.410 (53) 0
14	14	O	9	1.215386 (13)	4	118.915 (34)	5	171.468 (54) 0
15	15	O	10	1.229009 (14)	6	118.424 (35)	5	47.843 (55) 0
16	16	O	10	1.228699 (15)	6	117.185 (36)	5	-130.096 (56) 0
17	17	C	7	1.460684 (16)	1	128.292 (37)	2	-166.565 (57) 0
18	18	H	17	0.921158 (17)	7	109.960 (38)	1	156.284 (58) 0
19	19	H	17	0.999417 (18)	7	109.668 (39)	1	36.580 (59) 0
20	20	H	17	1.000129 (19)	7	112.597 (40)	1	-89.764 (60) 0
21	21	H	3	0.860628 (20)	4	120.806 (41)	5	-177.546 (61) 0
22	22	H	5	0.942765 (21)	6	124.091 (42)	1	178.406 (62) 0
23	23	H	7	0.925832 (22)	1	110.218 (43)	2	0.512 (63) 0

STOICHIOMETRY C7H6N4O6

SCF DONE: E(RHF) = -931.127125257

EIGENVALUES — -0.30129 -0.29658 0.12069 0.13943 0.18019

Estimated ionization potential: 8.08 eV

TOTAL ATOMIC CHARGES.

	1	Net Charge
1 C	5.799379	0.211
2 C	5.933513	0.066
3 C	6.081523	-0.082
4 C	5.915315	0.085
5 C	6.049286	-0.049
6 C	5.934450	0.066
7 N	7.374809	-0.375
8 N	6.829976	0.170
9 N	6.830918	0.169
10 N	6.839770	0.160
11 O	8.225055	-0.225
12 O	8.175589	-0.176
13 O	8.203996	-0.204
14 O	8.195592	-0.196
15 O	8.192980	-0.193
16 O	8.197565	-0.198
17 C	6.180449	-0.180
18 H	0.868422	0.132
19 H	0.884976	0.115
20 H	0.868150	0.132
21 H	0.845906	0.154
22 H	0.855156	0.145
23 H	0.717221	0.283

DIPOLE MOMENT (DEBYE): X=-2.7735 Y=-1.2510 Z=-2.1210 TOTAL= 3.7089

Bond Order: C2-N8: 1.28	V-mid: C2-N8: 0.172
C4-N9: 1.27	C4-N9: 0.185
C6-N10: 1.27	C6-N10: 0.164
N8-O11: 1.89	
N8-O12: 1.95	
N9-O13: 1.90	
N9-O14: 1.96	
N10-O15: 1.89	
N10-O16: 1.89	

-10.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
30.0
35.0
40.0
45.0
50.0
75.0

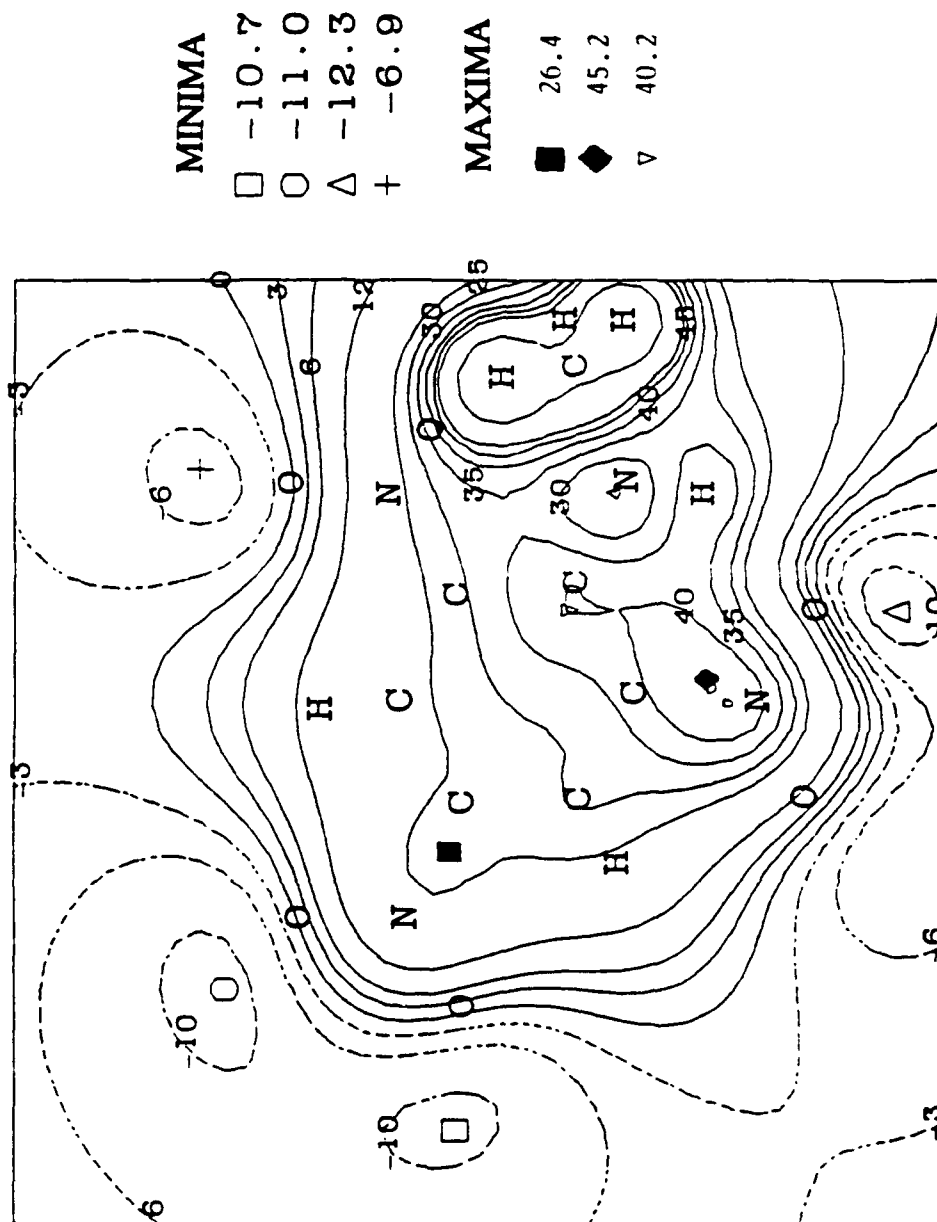
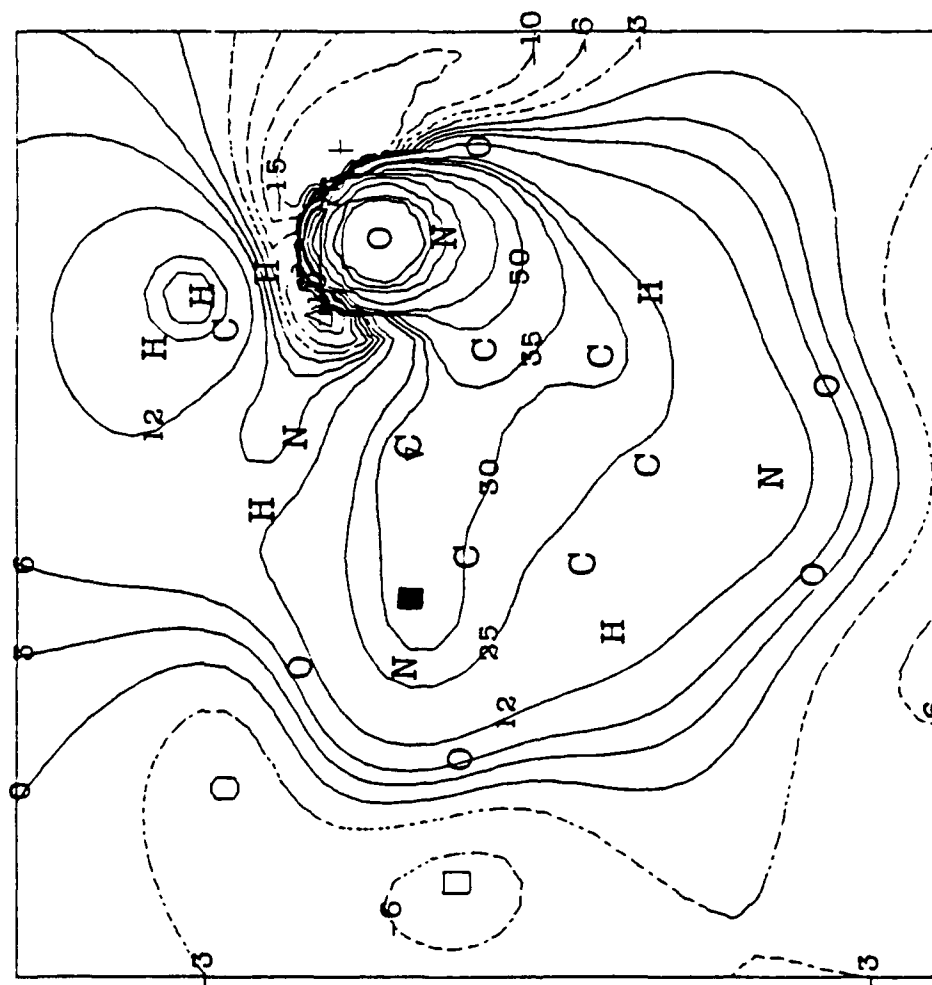


Figure FF-1. Calculated electrostatic potential, in kcal/mole, of N-methylpicramide, in the plane 1.75 Å above the N9 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-16.0
-10.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
30.0
35.0
50.0
75.0
150.0
300.0
600.0
1000.0



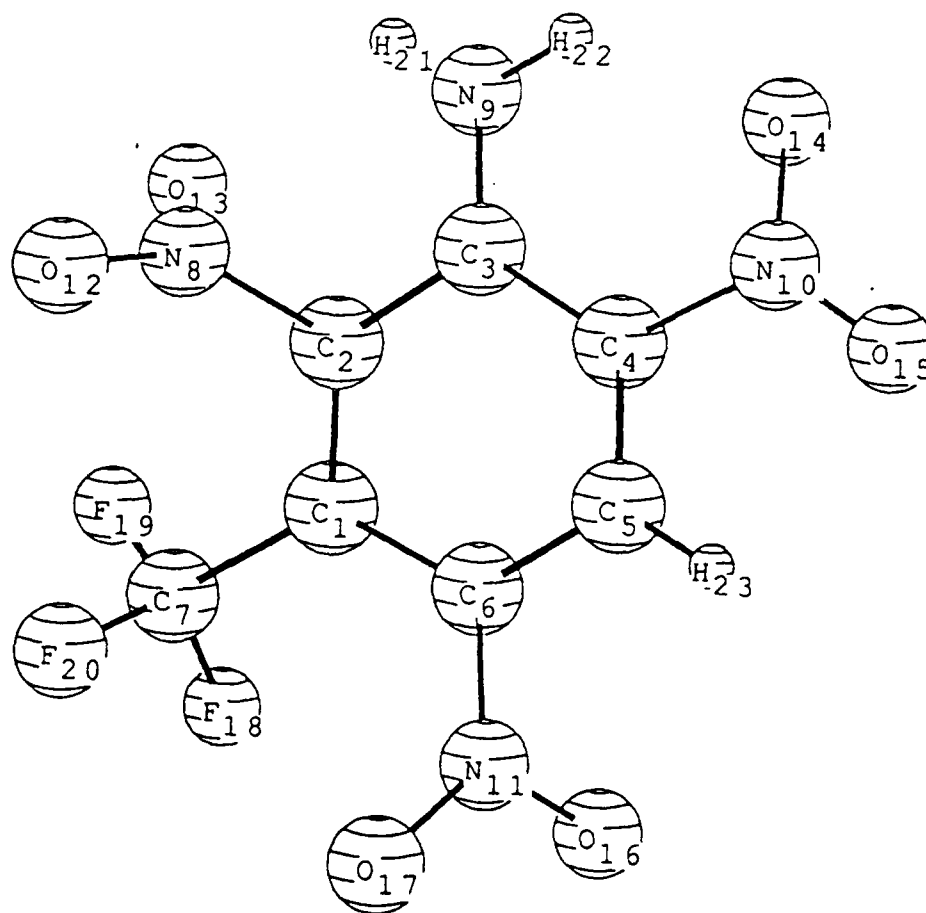
MINIMA		MAXIMA	
□	-6.7	■	32.0
○	-4.7	▽	34.5
△	-14.5		
+	-32.1		

Figure FF-2. Calculated electrostatic potential, in kcal/mole, of N-methylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX GG
3-TRIFLUOROMETHYL-2,4,6-TRINITROANILINE

The short distances between non-bonded hydrogens and oxygens are H21-O13 (2.21 Å), H22-O14 (1.94 Å), H23-O15 (2.36 Å) and H23-O16 (2.45 Å).

The N10 nitro group is rotated by only about 6°, while the N8 and N11 nitro groups are rotated by approximately 55° and 37°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	CENT	ATOM	N1	LENGTH	N2	ALPHA	N3	BETA	J
1	1	C							
2	2	C	1	1.377000 (1)					
3	3	C	2	1.423341 (2)	1	124.869 (23)			
4	4	C	3	1.414991 (3)	2	113.914 (24)	1	-3.607 (44)	0
5	5	C	4	1.368284 (4)	3	122.473 (25)	2	2.014 (45)	0
6	6	C	5	1.370912 (5)	4	120.672 (26)	3	-0.585 (46)	0
7	7	C	1	1.526463 (6)	2	120.289 (27)	3	-167.190 (47)	0
8	8	N	2	1.475356 (7)	3	116.159 (28)	4	172.719 (48)	0
9	9	N	3	1.328759 (8)	4	124.273 (29)	5	-178.928 (49)	0
10	10	N	4	1.459222 (9)	5	116.478 (30)	6	178.033 (50)	0
11	11	N	6	1.464138 (10)	5	117.502 (31)	4	-176.072 (51)	0
12	12	O	8	1.219998 (11)	2	116.274 (32)	3	-123.853 (52)	0
13	13	O	8	1.224792 (12)	2	118.839 (33)	3	55.066 (53)	0
14	14	O	10	1.217181 (13)	4	119.193 (34)	5	173.113 (54)	0
15	15	O	10	1.210136 (14)	4	118.346 (35)	5	-6.139 (55)	0
16	16	O	11	1.226621 (15)	6	117.128 (36)	5	-35.466 (56)	0
17	17	O	11	1.220246 (16)	6	118.049 (37)	5	140.211 (57)	0
18	18	F	7	1.336189 (17)	1	111.715 (38)	2	142.156 (58)	0
19	19	F	7	1.335440 (18)	1	111.454 (39)	2	24.746 (59)	0
20	20	F	7	1.327102 (19)	1	112.764 (40)	2	-96.090 (60)	0
21	21	H	9	0.828794 (20)	3	121.524 (41)	4	173.273 (61)	0
22	22	H	9	0.916242 (21)	3	118.686 (42)	4	0.225 (62)	0
23	23	H	5	0.930860 (22)	4	121.966 (43)	3	179.783 (63)	0

STOICHIOMETRY C7H3F3N4O6

SCF DONE: E(RHF) = -1226.15046963

EIGENVALUES — -0.32830 -0.32454 -0.32219 -0.31111 0.10521

Estimated ionization potential: 8.47 ev

TOTAL ATOMIC CHARGES.

		1	Net Charge
1	C	5.984284	0.016
2	C	5.929704	0.070
3	C	5.784771	0.215
4	C	5.931482	0.069
5	C	6.056998	-0.057
6	C	5.915220	0.085
7	C	5.508179	0.492
8	N	6.832628	0.167
9	N	7.547599	-0.548
10	N	6.820424	0.180
11	N	6.831440	0.169
12	O	8.177611	-0.178
13	O	3.199445	-0.199
14	O	8.220131	-0.220
15	O	8.182812	-0.183
16	O	8.190944	-0.191
17	O	8.187893	-0.188
18	F	9.152070	-0.152
19	F	9.156847	-0.157
20	F	9.140736	-0.141
21	H	0.700174	0.300
22	H	0.700424	0.300
23	H	0.848186	0.152

DIPOLE MOMENT (DEBYE): X= 0.6634 Y= 0.4913 Z= 2.8702 TOTAL= 2.9871

Bond Order: C2-N8: 1.23

C4-N10: 1.27

C6-N11: 1.25

N8-O12: 1.94

N8-O13: 1.91

N10-O14: 1.95

N10-O15: 1.99

N11-O16: 1.91

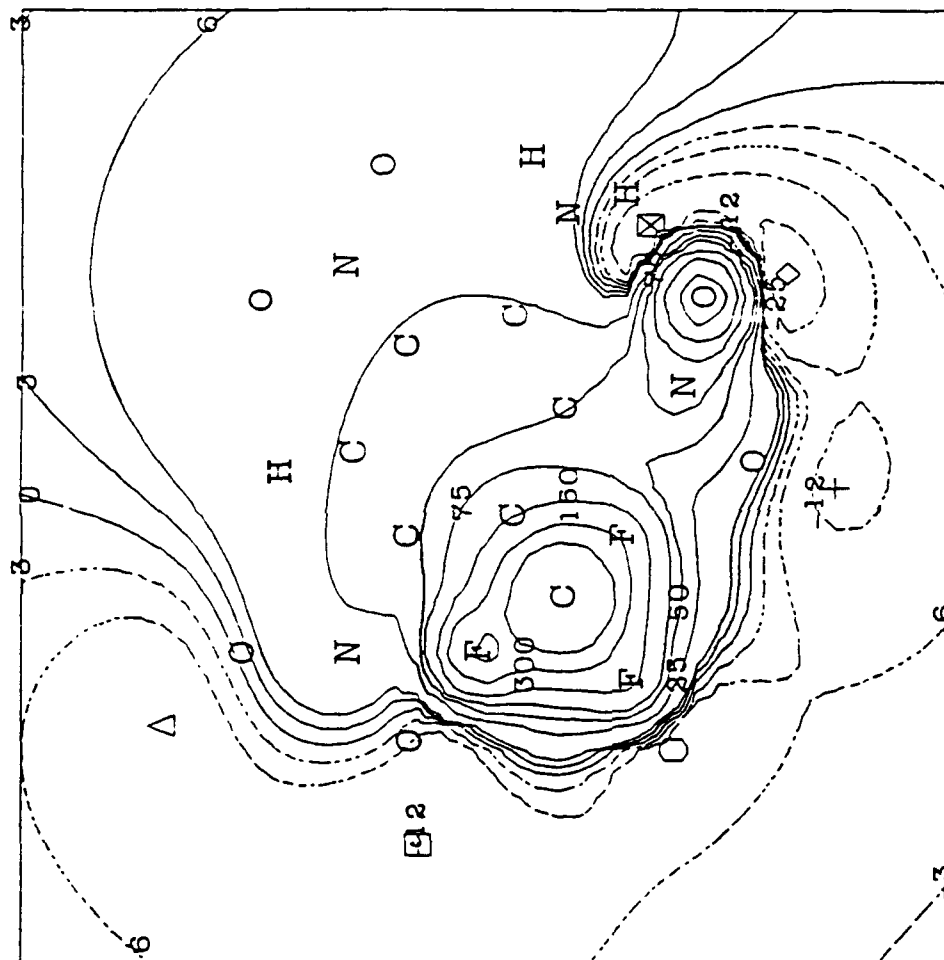
N11-O17: 1.94

V-mid: C2-N8: 0.170

C4-N10: 0.181

C6-N11: 0.184

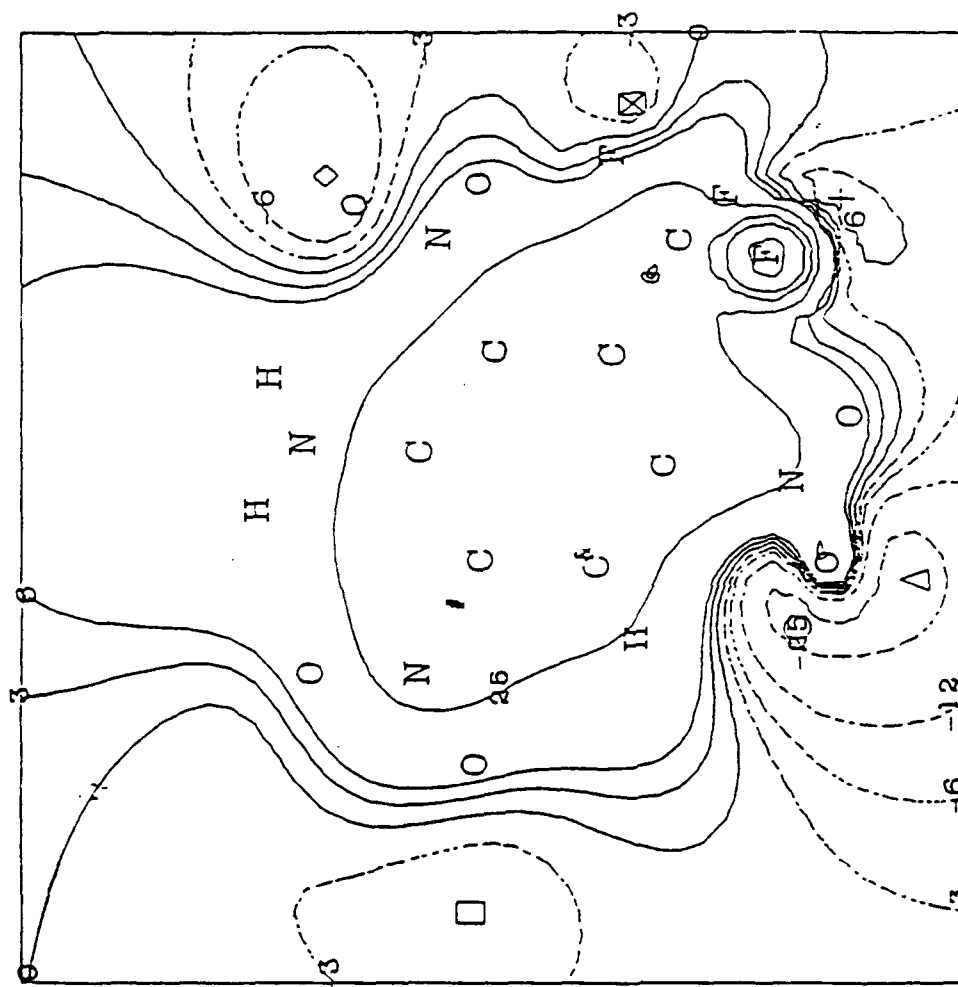
-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0
300.0
600.0



MINIMA	
□	-12.036
○	-10.153
△	-9.827
+	-13.811
◇	-38.466
⊗	-23.168

Figure GG-1. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,5-trinitroaniline, in the plane 1.75Å above the N11 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
25.0
50.0
75.0
150.0



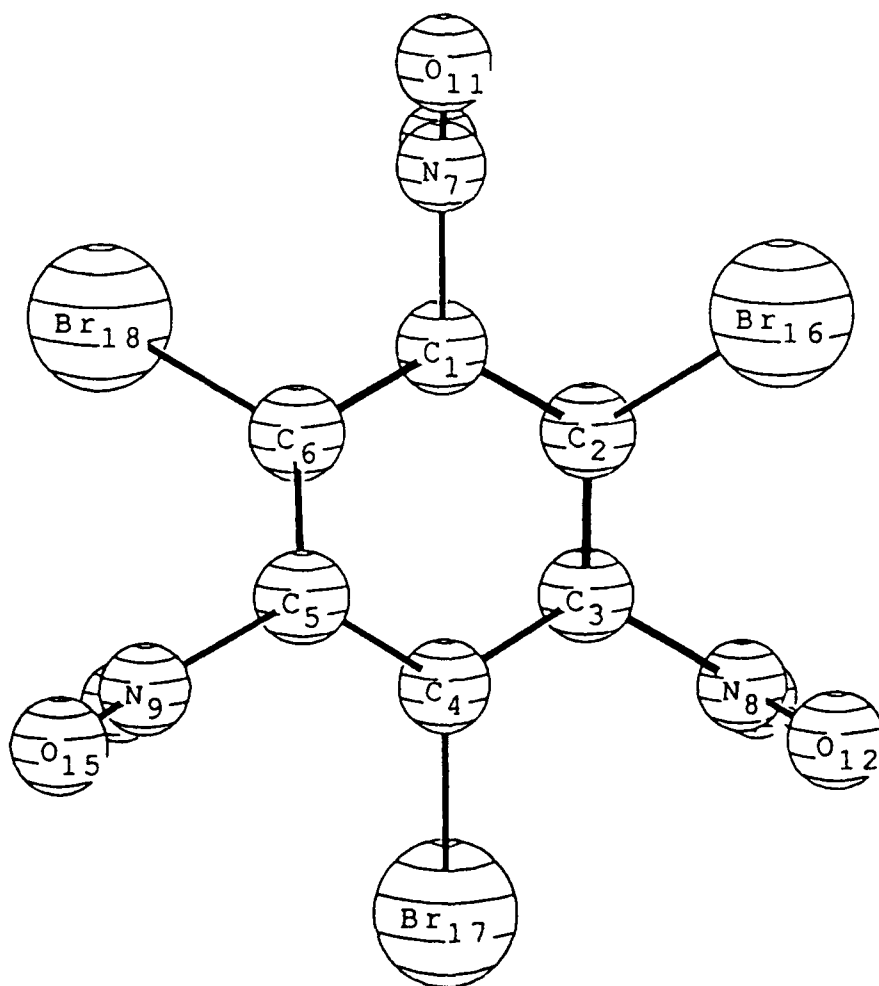
MINIMA	
□	-4.819
○	-30.422
△	-32.022
+	-7.725
◇	-10.768
⊗	-5.146

MAXIMA	
⋈	+34.613
#	+36.006
@	+50.445

Figure GG-2. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,5-trinitroaniline, in the plane 1.75Å above the N10 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX HH
1,3,5-TRIBROMO-2,4,6-TRINITROBENZENE

All three nitro groups are essentially perpendicular to the mean plane of the benzene ring.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.393000(1)				
3	3	C	2	1.348241(2)	1	118.314(18)		
4	4	C	3	1.391096(3)	2	123.257(19)	1	-1.997(34) 0
5	5	C	4	1.391208(4)	3	116.077(20)	2	1.075(35) 0
6	6	C	5	1.348499(5)	4	123.244(21)	3	0.999(36) 0
7	7	N	1	1.478230(6)	2	119.616(22)	3	-179.033(37) 0
8	8	N	3	1.493504(7)	2	118.852(23)	1	177.130(38) 0
9	9	N	5	1.493336(8)	4	117.850(24)	3	-178.112(39) 0
10	10	O	7	1.217902(9)	1	115.518(25)	2	90.887(40) 0
11	11	O	7	1.218270(10)	1	115.515(26)	2	-89.181(41) 0
12	12	O	8	1.214312(11)	3	114.720(27)	2	90.325(42) 0
13	13	O	8	1.187091(12)	3	118.131(28)	2	-91.002(43) 0
14	14	O	9	1.214241(13)	5	114.710(29)	6	90.276(44) 0
15	15	O	9	1.187406(14)	5	118.122(30)	6	-90.997(45) 0
16	16	Br	2	1.872735(15)	3	121.701(31)	4	175.775(46) 0
17	17	Br	4	1.856453(16)	3	121.948(32)	2	-178.987(47) 0
18	18	Br	6	1.872691(17)	5	121.677(33)	4	175.825(48) 0

STOICHIOMETRY C6Br3N3O6

SCF DONE: E(RHF) = -8512.21818058

Alpha eigenvalues — -0.34212 -0.33284 -0.33243 -0.33020 0.12972

Estimated ionization potential: 8.99 ev

Total atomic charges:

1
 1 C 0.102297
 2 C -0.031984
 3 C 0.092852
 4 C -0.027379
 5 C 0.092918
 6 C -0.031978
 7 N 0.175023
 8 N 0.190006
 9 N 0.189896
 10 O -0.173694
 11 O -0.173812
 12 O -0.186747
 13 O -0.176726
 14 O -0.186619
 15 O -0.176734
 16 Br 0.103060
 17 Br 0.116546
 18 Br 0.103074

Dipole moment (Debye):

X= -0.0006 Y= 0.0299 Z= 0.0019 Tot= 0.0299

Bond Order: C1-N7: 1.22

C3-N8: 1.18

C5-N9: 1.18

N7-O10: 1.95

N7-O11: 1.95

N8-O12: 1.97

N8-O13: 2.10

N9-O14: 1.97

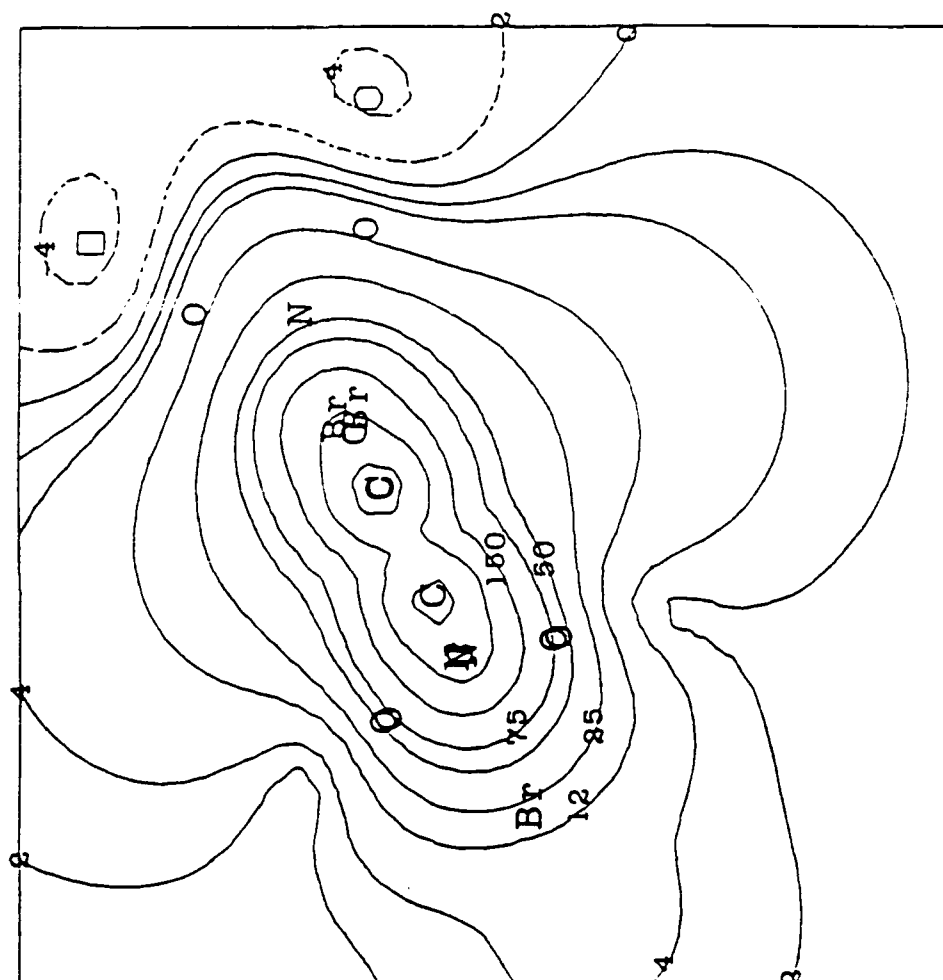
N9-O15: 2.10

V-mid: C1-N7: 0.198

C3-N8: 0.201

C5-N9: 0.201

-4.0
-2.0
0.0
2.0
4.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0



MINIMA
□ -4.4
○ -4.3

Figure HH-1. Calculated electrostatic potential, in kcal/mole, of 1,3,5-tribromo-2,4,6-trinitrobenzene, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-4.0
-2.0
0.0
2.0
4.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0

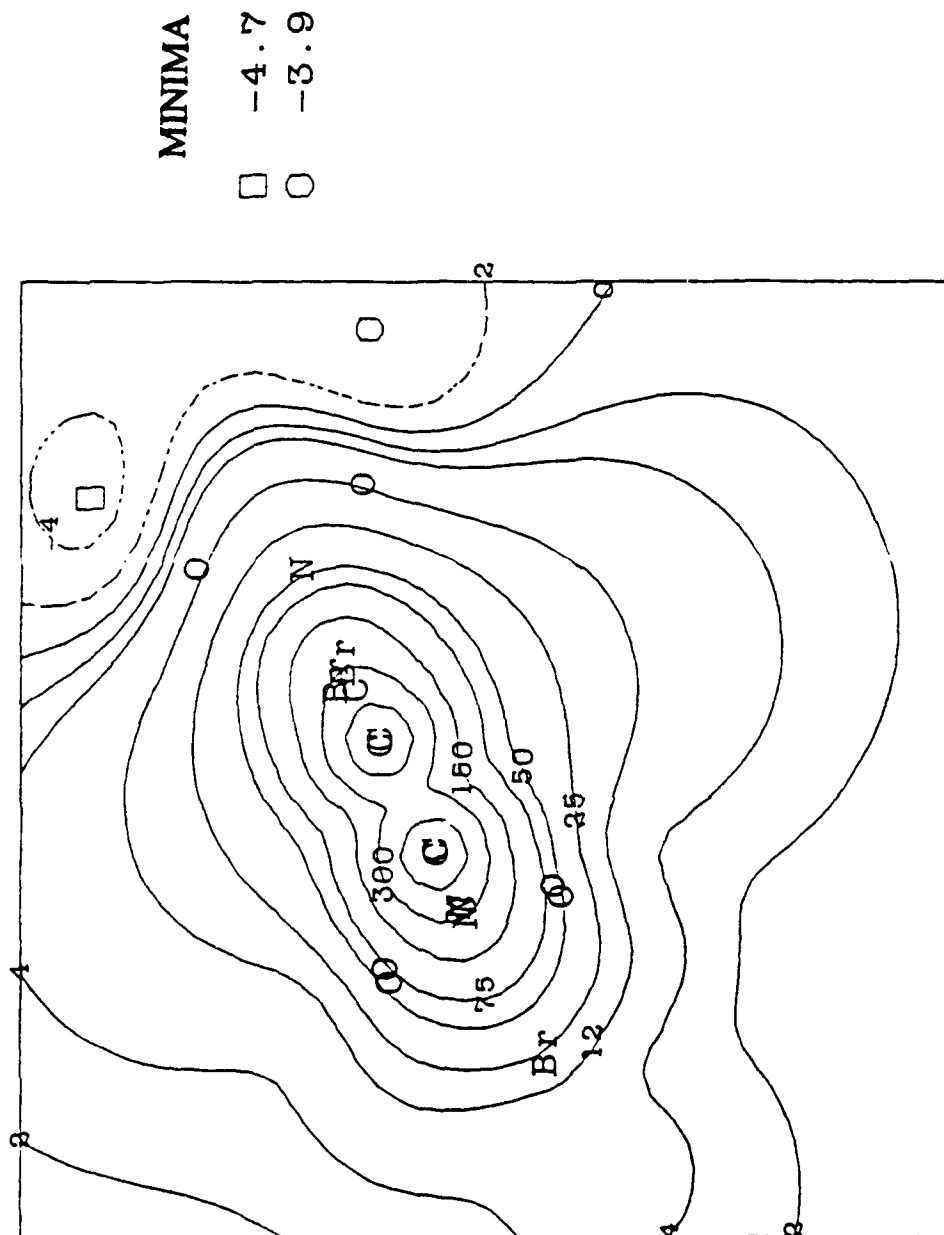
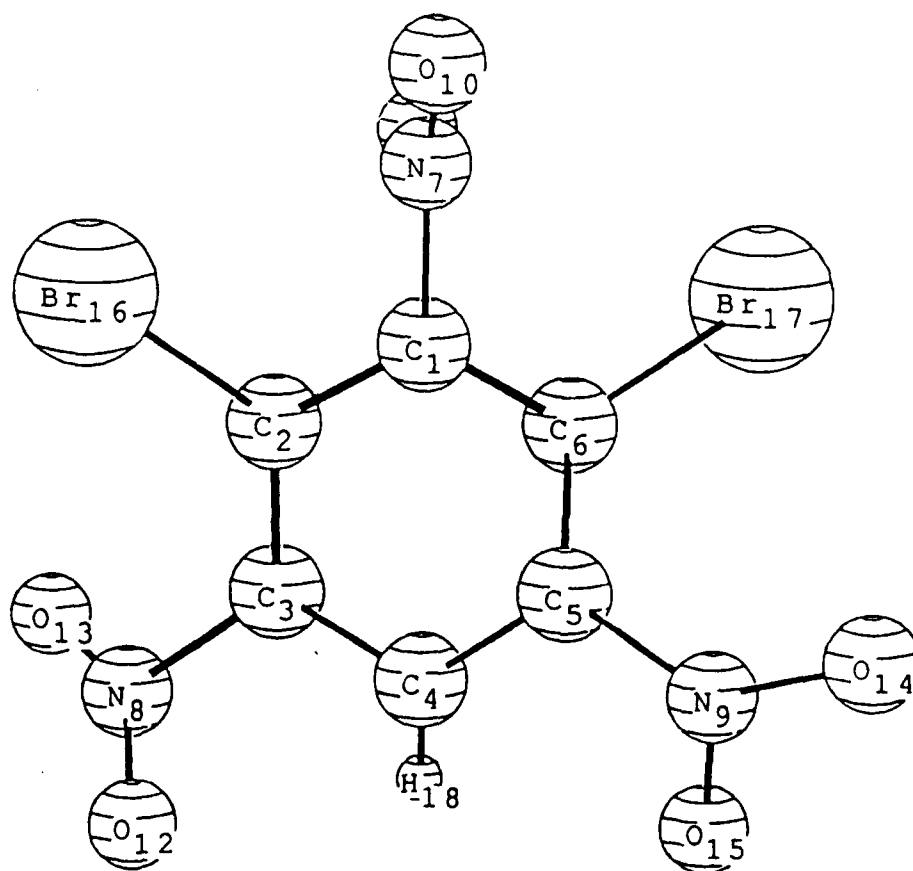


Figure HH-2. Calculated electrostatic potential, in kcal/mole, of 1,3,5-tribromo-2,4,6-trinitrobenzene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX II
2,4-DIBROMO-1,3,5-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H18-O12 (2.44 Å) and H18-O15 (2.44 Å).

The N8 and N9 nitro groups are rotated out of the mean plane of the benzene ring by 30°, while the N7 nitro group is approximately perpendicular to the ring (~95°).



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.380000(1)				
3	3	C	2	1.390498(2)	1	116.357(18)		
4	4	C	3	1.382818(3)	2	122.441(19)	1	1.111(34)
5	5	C	4	1.382818(4)	3	118.020(20)	2	-0.584(35)
6	6	C	5	1.390498(5)	4	122.441(21)	3	-0.584(36)
7	7	N	1	1.480000(6)	2	117.814(22)	3	179.466(37)
8	8	N	3	1.479386(7)	4	115.151(23)	5	178.818(38)
9	9	N	5	1.479386(8)	4	115.151(24)	3	178.818(39)
10	10	O	7	1.210060(9)	1	117.034(25)	2	94.656(40)
11	11	O	7	1.210740(10)	1	117.018(26)	2	-85.379(41)
12	12	O	8	1.208234(11)	3	116.904(27)	4	29.845(42)
13	13	O	8	1.211220(12)	3	118.132(28)	4	-149.941(43)
14	14	O	9	1.211322(13)	5	118.154(29)	4	-149.989(44)
15	15	O	9	1.207948(14)	5	116.948(30)	4	29.831(45)
16	16	Br	2	1.891338(15)	3	125.206(31)	4	-175.584(46)
17	17	Br	6	1.891866(16)	5	125.196(32)	4	-175.555(47)
18	18	H	4	0.807000(17)	5	120.990(33)	6	179.416(48)

STOICHIOMETRY C6HBr2N3O6

SCF DONE: E(RHF) = -5953.87892238

Alpha eigenvalues — -0.32804 -0.32390 -0.32381 0.10685 0.12158

Estimated ionization potential: 8.82 ev

Total atomic charges:

1
 1 C 0.100374
 2 C -0.025497
 3 C 0.115873
 4 C -0.105965
 5 C 0.115836
 6 C -0.025324
 7 N 0.178433
 8 N 0.181801
 9 N 0.181819
 10 O -0.179373
 11 O -0.179622
 12 O -0.187011
 13 O -0.185362
 14 O -0.185495
 15 O -0.187001
 16 Br 0.115126
 17 Br 0.115026
 18 H 0.156362

Dipole moment (Debye):

X= -0.0043 Y= -0.2721 Z= -0.0025 Tot= 0.2721

Bond Order: C1-N7: 1.21	V-mid: C1-N7: 0.199
C3-N8: 1.22	C3-N8: 0.213
C5-N9: 1.22	C5-N9: 0.213
N7-O10: 1.99	
N7-O11: 1.98	
N8-O12: 2.00	
N8-O13: 1.99	
N9-O14: 1.99	
N9-O15: 2.00	

-25.0
-12.0
-4.0
-2.0
0.0
2.0
4.0
12.0
25.0
35.0
50.0
75.0
150.0
300.0
600.0
1000.0

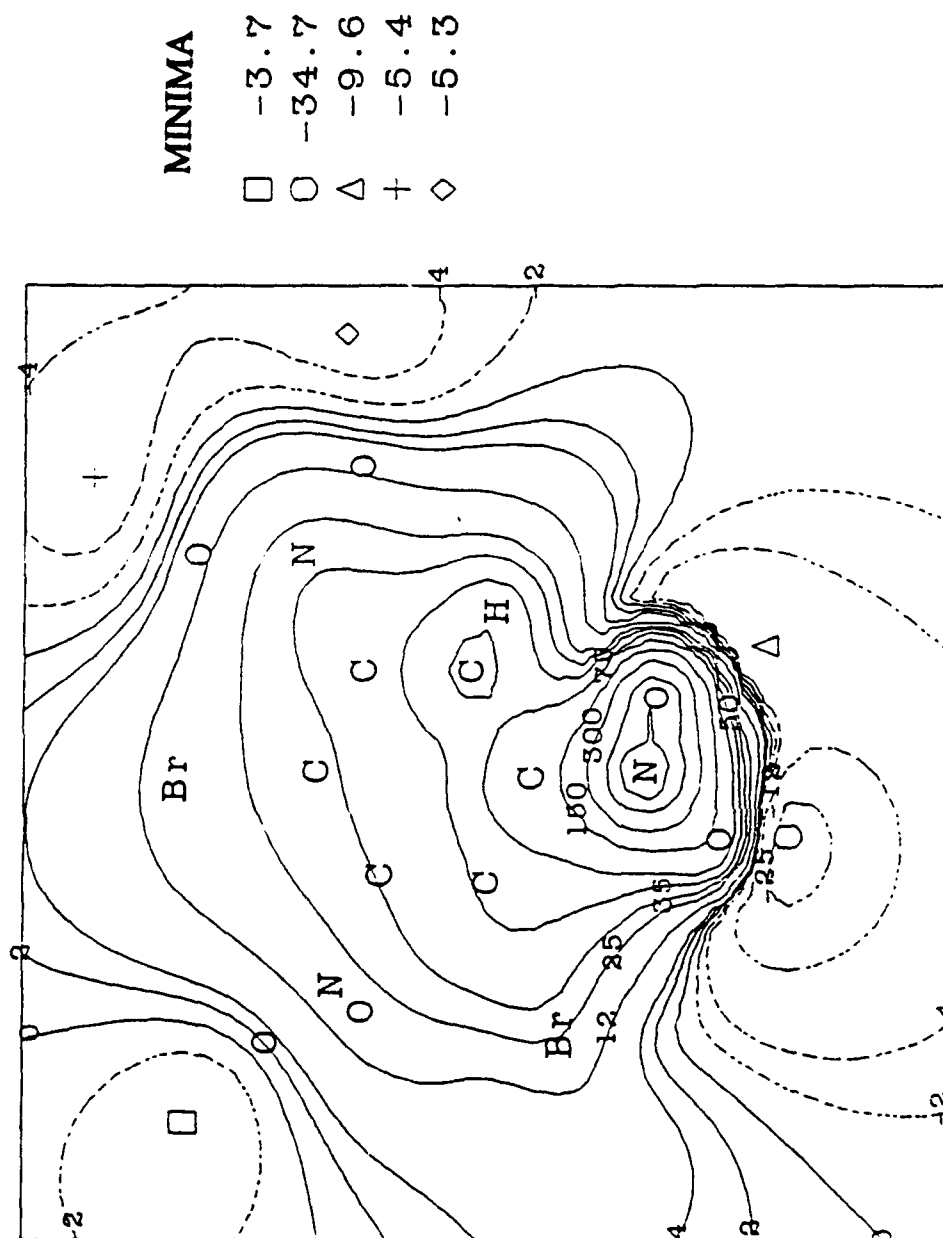


Figure II-1. Calculated electrostatic potential, in kcal/mole, of 2,4-dibromo-1,3,5-trinitrobenzene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-4.0
-2.0
0.0
2.0
4.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0

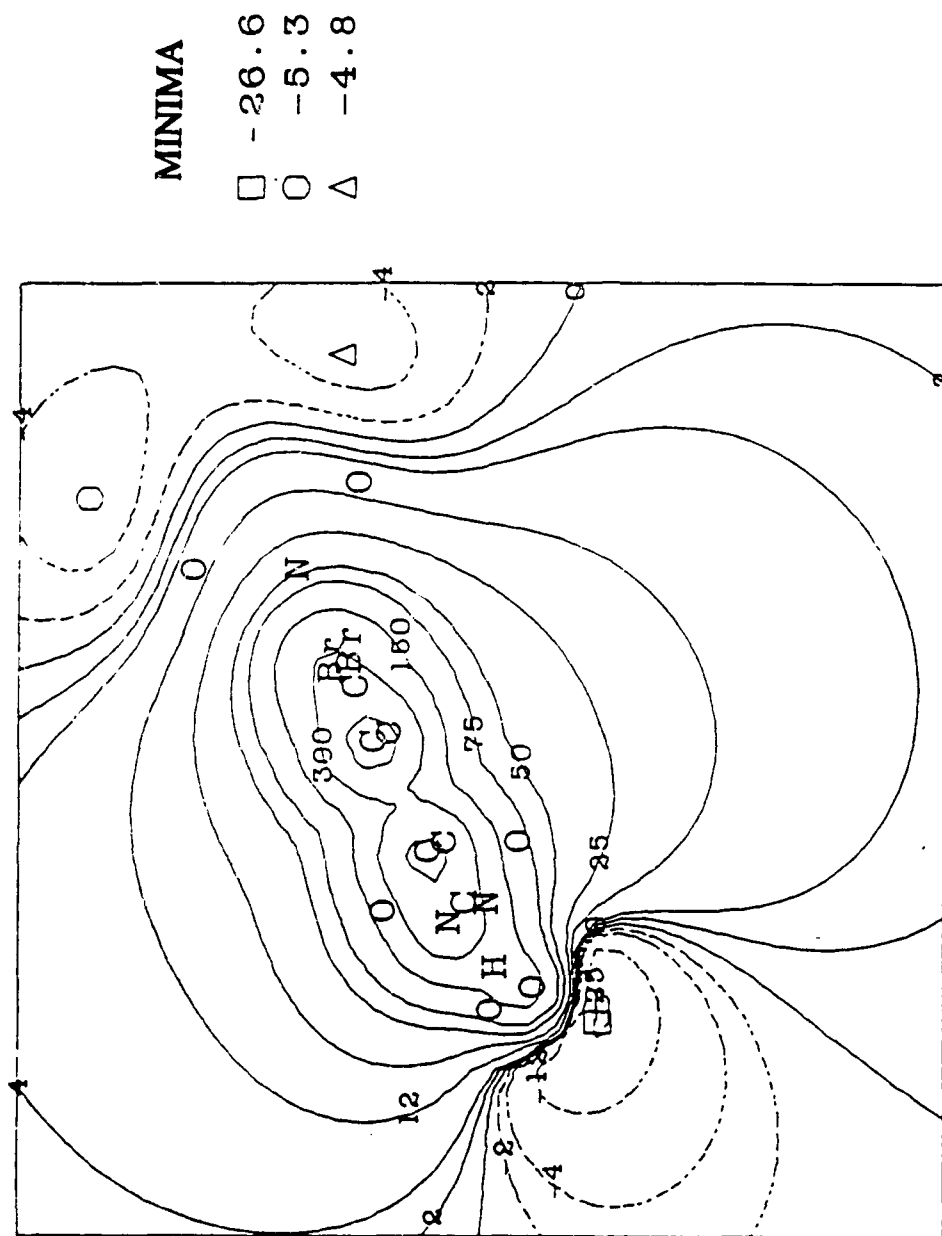
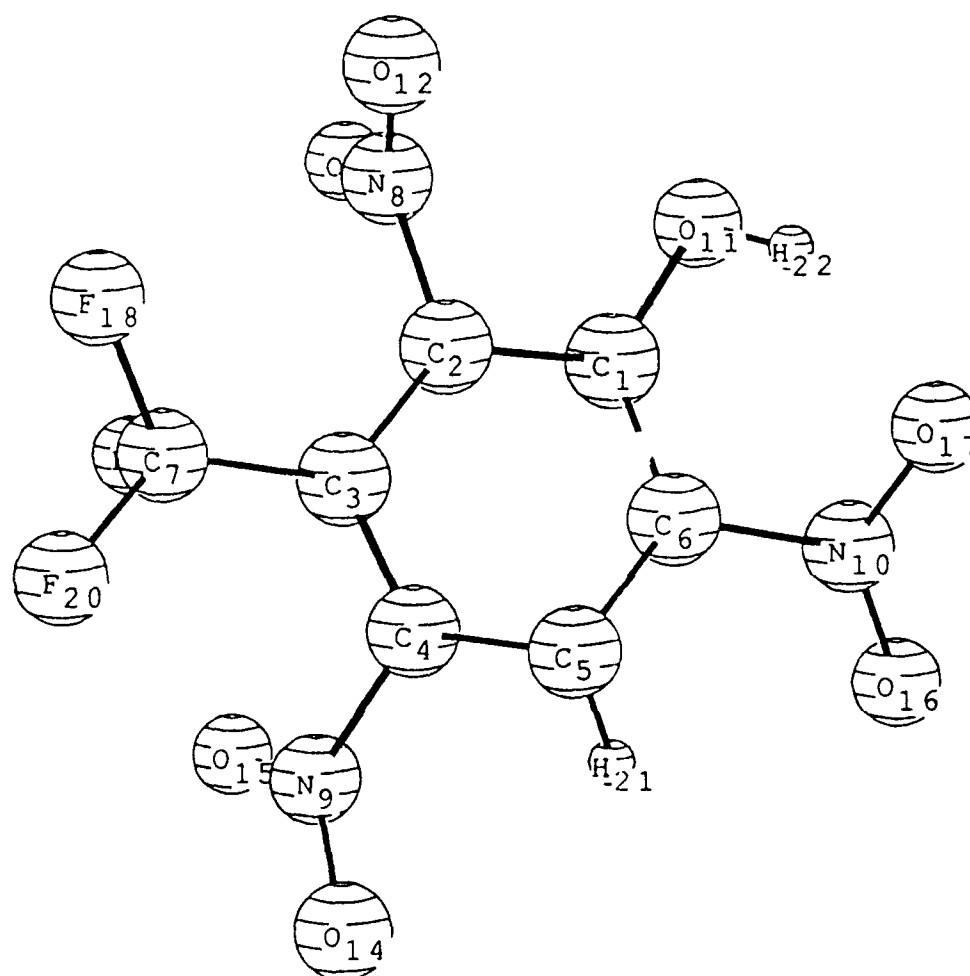


Figure II-2. Calculated electrostatic potential, in kcal/mole, of 2,4-dibromo-1,3,5-trinitrobenzene, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX JJ
3-TRIFLUOROMETHYL-2,4,6-TRINITROPHENOL

The short distances between non-bonded hydrogens and oxygens are H21-O16 (2.46 Å), H21-O14 (2.51 Å) and H22-O17 (1.90 Å).

The N10 nitro group is essentially planar, while the N8 and N9 nitro groups are rotated out of the plane by about 75° and 47°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.404000(1)					
3	3	C	2	1.377935(2)	1	123.606(22)			
4	4	C	3	1.389770(3)	2	116.643(23)	1	0.328(42)	0
5	5	C	4	1.371750(4)	3	122.259(24)	2	1.301(43)	0
6	6	C	5	1.372874(5)	4	119.185(25)	3	-1.787(44)	0
7	7	C	3	1.528478(6)	4	122.350(26)	5	-174.260(45)	0
8	8	N	2	1.470356(7)	3	121.911(27)	4	179.191(46)	0
9	9	N	4	1.474082(8)	5	115.956(28)	6	176.116(47)	0
10	10	N	6	1.473645(9)	5	117.657(29)	4	-177.434(48)	0
11	11	O	1	1.326126(10)	2	117.062(30)	3	178.427(49)	0
12	12	O	8	1.215598(11)	2	117.138(31)	3	105.300(50)	0
13	13	O	8	1.209973(12)	2	117.510(32)	3	-75.519(51)	0
14	14	O	9	1.214281(13)	4	117.277(33)	5	46.276(52)	0
15	15	O	9	1.217971(14)	4	117.477(34)	5	-131.208(53)	0
16	16	O	10	1.199587(15)	6	118.296(35)	5	1.764(54)	0
17	17	O	10	1.221103(16)	6	117.472(36)	5	-177.931(55)	0
18	18	F	7	1.331131(17)	3	110.958(37)	4	150.137(56)	0
19	19	F	7	1.316372(18)	3	111.025(38)	4	-90.023(57)	0
20	20	F	7	1.310814(19)	3	111.626(39)	4	31.997(58)	0
21	21	H	5	0.972101(20)	4	115.616(40)	3	-177.019(59)	0
22	22	H	11	0.819230(21)	1	107.493(41)	6	-11.126(60)	0

SCF DONE: E(RHF) = -1245.86368404

Alpha eigenvalues — -0.35002 -0.34604 -0.32175 -0.31498 0.10080

Estimated ionization potential: 8.58 ev

Total atomic charges:

1
 1 C 0.203108
 2 C 0.086656
 3 C 0.006774
 4 C 0.093541
 5 C -0.047036
 6 C 0.061299
 7 C 0.506982
 8 N 0.184475
 9 N 0.174856
 10 N 0.185986
 11 O -0.362201
 12 O -0.179356
 13 O -0.183966
 14 O -0.186585
 15 O -0.187443
 16 O -0.166619
 17 O -0.225928
 18 F -0.156473
 19 F -0.145043
 20 F -0.154374
 21 H 0.146811
 22 H 0.344536

Dipole moment (Debye):

X= 2.1028 Y= 0.6998 Z= -0.3858 Tot= 2.2495

Bond Order:	C2-N8: 1.24	V-mid: C2-N8: 0.195
	C4-N9: 1.23	C4-N9: 0.193
	C6-N10: 1.23	C6-N10: 0.177
	N8-O12: 1.96	
	N8-O13: 1.99	
	N9-O14: 1.97	
	N9-O15: 1.95	
	N10-O16: 2.04	
	N10-O17: 1.93	

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0

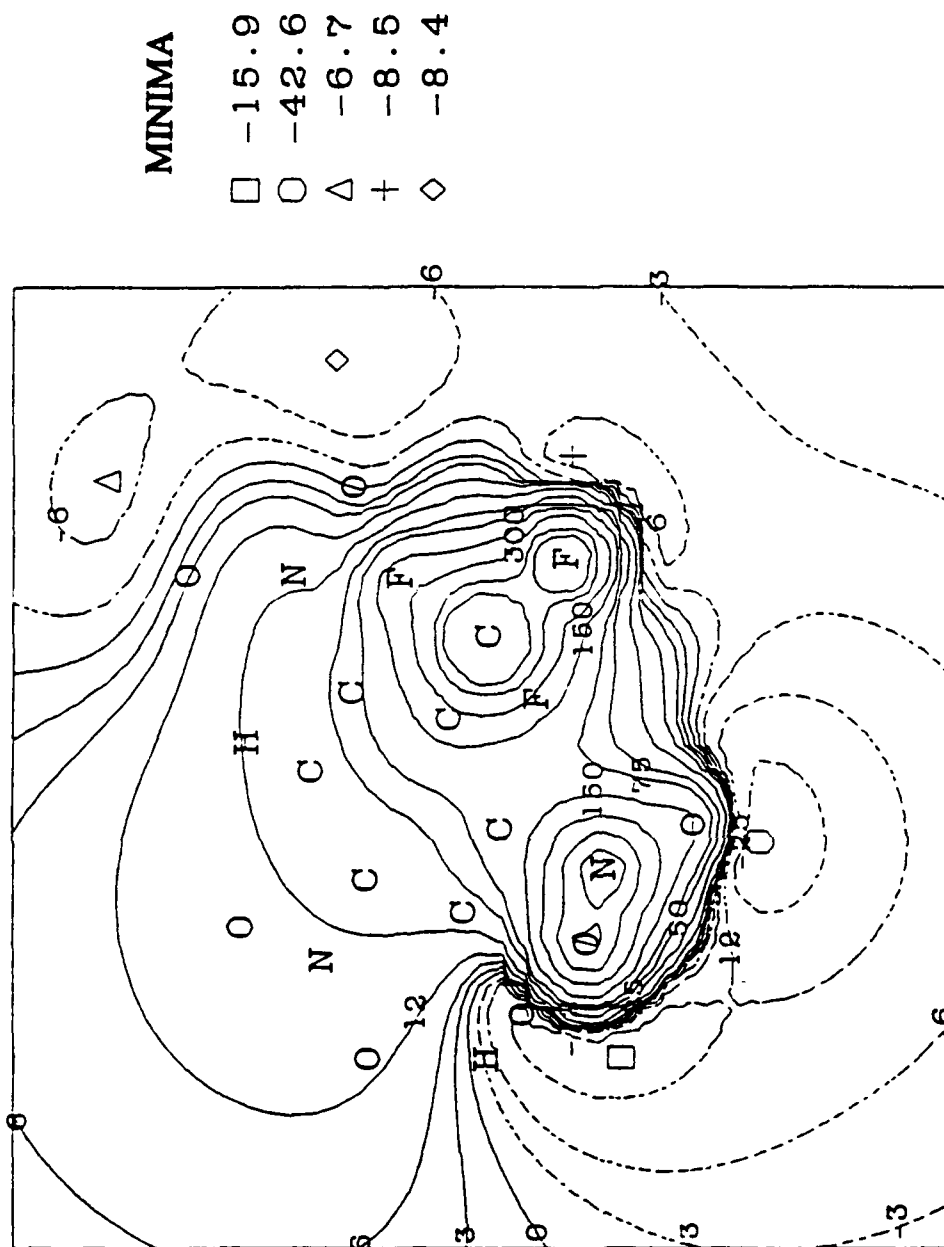
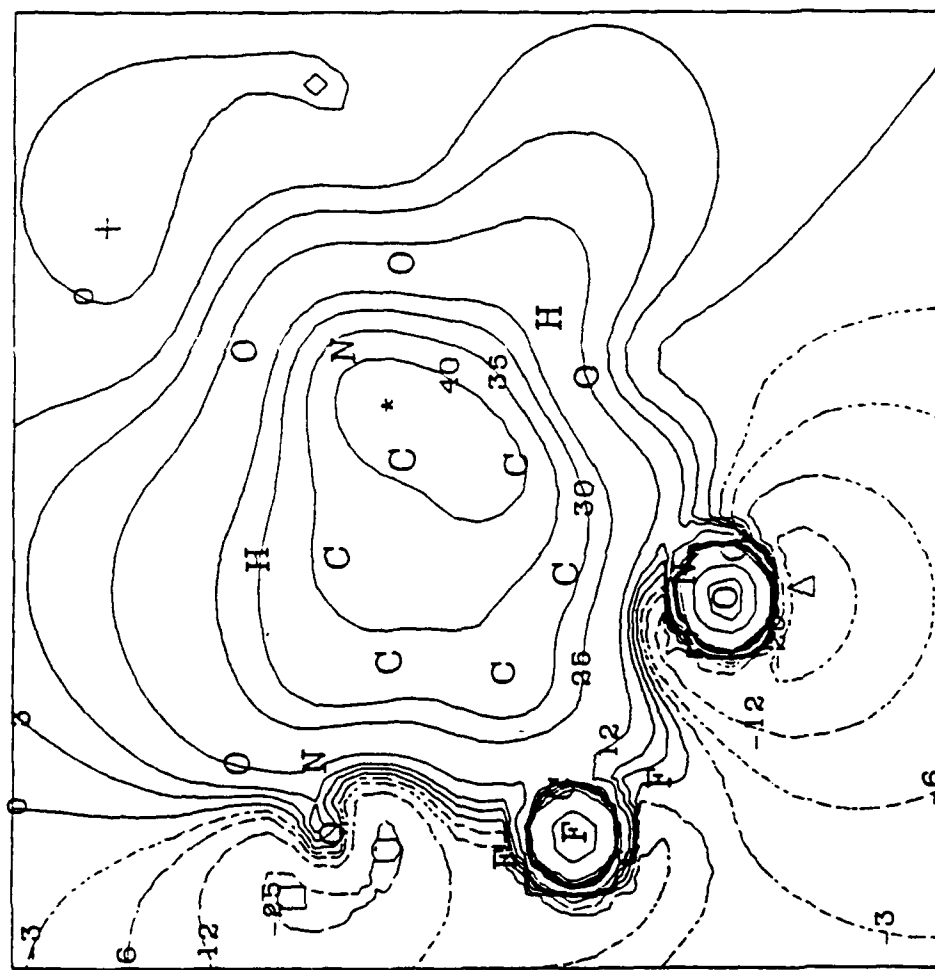


Figure JJ-1. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,6-trinitrophenol, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
30.0
36.0
40.0
50.0
150.0
300.0



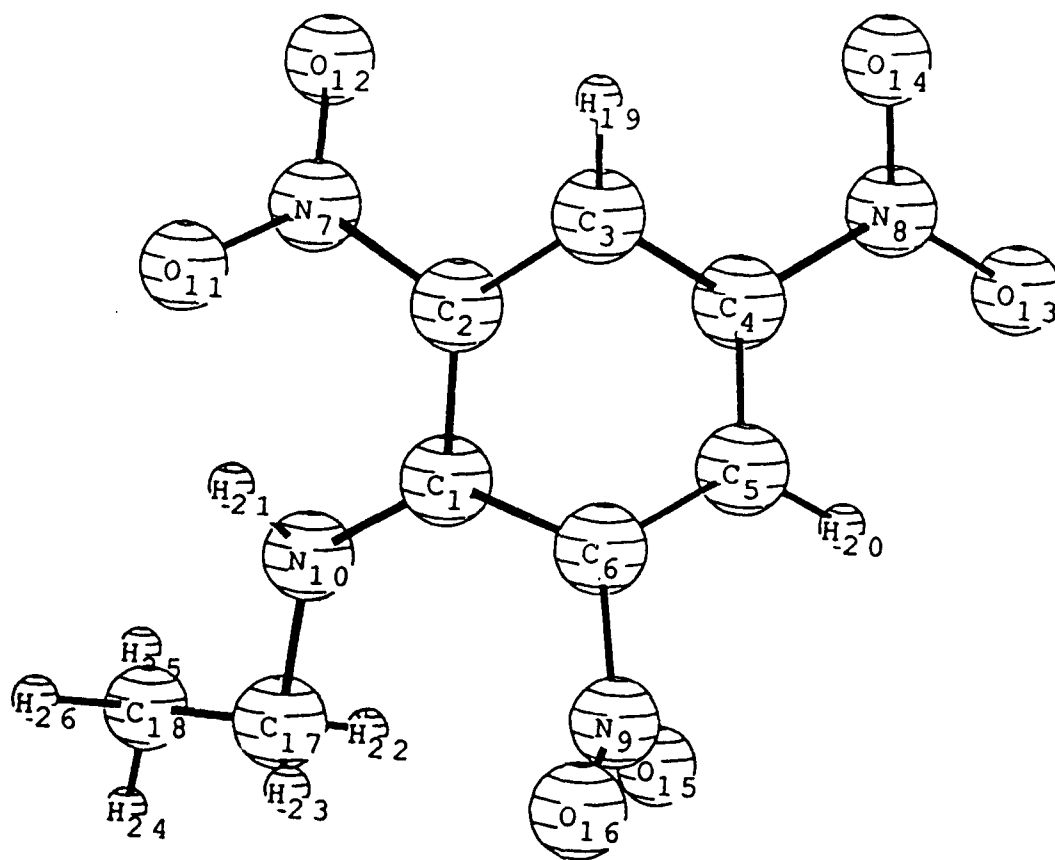
MAXIMA	
□	-28.9
○	-28.7
△	-39.1
+	-0.6
◇	-0.1
MINIMA	
*	43.2

Figure JJ-2. Calculated electrostatic potential, in kcal/mole, of 3-trifluoromethyl-2,4,6-trinitrophenol, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX KK N-ETHYLPICRAMIDE

The short distances between non-bonded hydrogens and oxygens are H21-O11 (1.86 Å), H19-O12 (2.30 Å), H20-O13 (2.43 Å) and H19-O14 (2.42 Å).

The N7 and N9 nitro groups are rotated by approximately 16° and 63°, while the N8 nitro group is almost planar.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C	1	1.452000(1)				
3	3	C	2	1.383366(2)	1	125.488(26)		
4	4	C	3	1.375288(3)	2	117.056(27)	1	0.466(50)
5	5	C	4	1.385204(4)	3	122.328(28)	2	-1.217(51)
6	6	C	5	1.357979(5)	4	118.178(29)	3	-0.371(52)
7	7	N	2	1.444456(6)	3	113.303(30)	4	-175.605(53)
8	8	N	4	1.472789(7)	5	119.316(31)	6	-178.995(54)
9	9	N	6	1.474800(8)	5	114.736(32)	4	-173.377(55)
10	10	N	1	1.311624(9)	2	122.669(33)	3	-177.952(56)
11	11	O	7	1.219191(10)	2	119.271(34)	1	16.622(57)
12	12	O	7	1.218956(11)	2	119.482(35)	1	-164.796(58)
13	13	O	8	1.223478(12)	4	117.155(36)	3	-175.437(59)
14	14	O	8	1.227899(13)	4	118.349(37)	3	2.636(60)
15	15	O	9	1.217938(14)	6	117.621(38)	1	118.997(61)
16	16	O	9	1.206604(15)	6	117.433(39)	1	-63.474(62)
17	17	C	10	1.457236(16)	1	127.715(40)	2	162.809(63)
18	18	C	17	1.519795(17)	10	107.228(41)	1	-150.949(64)
19	19	H	3	0.959378(18)	4	121.418(42)	5	178.855(65)
20	20	H	5	0.960549(19)	4	121.006(43)	3	179.444(66)
21	21	H	10	0.891037(20)	1	107.469(44)	2	-13.213(67)
22	22	H	17	0.960053(21)	10	109.853(45)	1	-31.507(68)
23	23	H	17	0.959400(22)	10	110.263(46)	1	89.275(69)
24	24	H	18	0.959927(23)	17	109.454(47)	10	179.758(70)
25	25	H	18	0.960684(24)	17	109.538(48)	10	59.752(71)
26	26	H	18	0.959818(25)	17	109.486(49)	10	-60.235(72)

STOICHIOMETRY C8H8N4O6

SCF DONE: E(RHF) = -970.057729827 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.29392 0.12726 0.14741 0.19115 0.23185

Estimated ionization potential: 8.01 ev

Total atomic charges:

1
 1 C 0.199520
 2 C 0.057593
 3 C -0.047819
 4 C 0.077816
 5 C -0.049395
 6 C 0.065943
 7 N 0.168615
 8 N 0.167424
 9 N 0.171636
 10 N -0.404492
 11 O -0.229021
 12 O -0.188108
 13 O -0.200677
 14 O -0.201120
 15 O -0.199962
 16 O -0.198314
 17 C -0.046327
 18 C -0.293763
 19 H 0.151310
 20 H 0.141052
 21 H 0.291566
 22 H 0.112157
 23 H 0.120304
 24 H 0.113478
 25 H 0.110211
 26 H 0.110374

Dipole moment (Debye):

X= -3.7803 Y= 0.2872 Z= -0.1971 Tot= 3.7963

V-mid: C2-N7: 0.167

C4-N8: 0.176

C6-N9: 0.172

Bond Order: C2-N7: 1.32

C4-N8: 1.24

C6-N9: 1.24

N7-O11: 1.94

N7-O12: 1.94

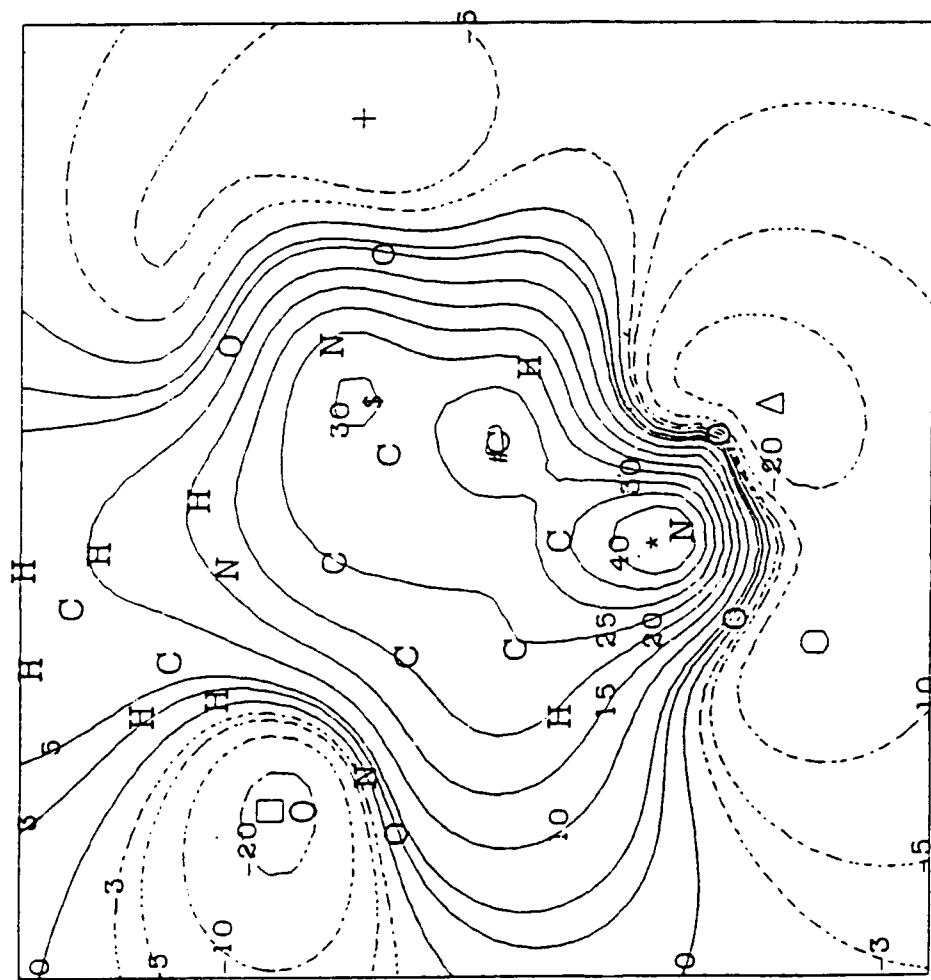
N8-O13: 1.92

N8-O14: 1.90

N9-O15: 1.95

N9-O16: 2.00

-20.0
-10.0
-5.0
-3.0
0.0
3.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0



MINIMA	
□	-23.9
○	-18.1
△	-33.2
+	-7.5
MAXIMA	
*	-46.0
#	-35.6
\$	-30.5

Figure KK-1. Calculated electrostatic potential, in kcal/mole, of N-ethylpicramide, in the plane 1.75 Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
30.0
40.0
50.0
100.0
300.0
500.0
1000.0

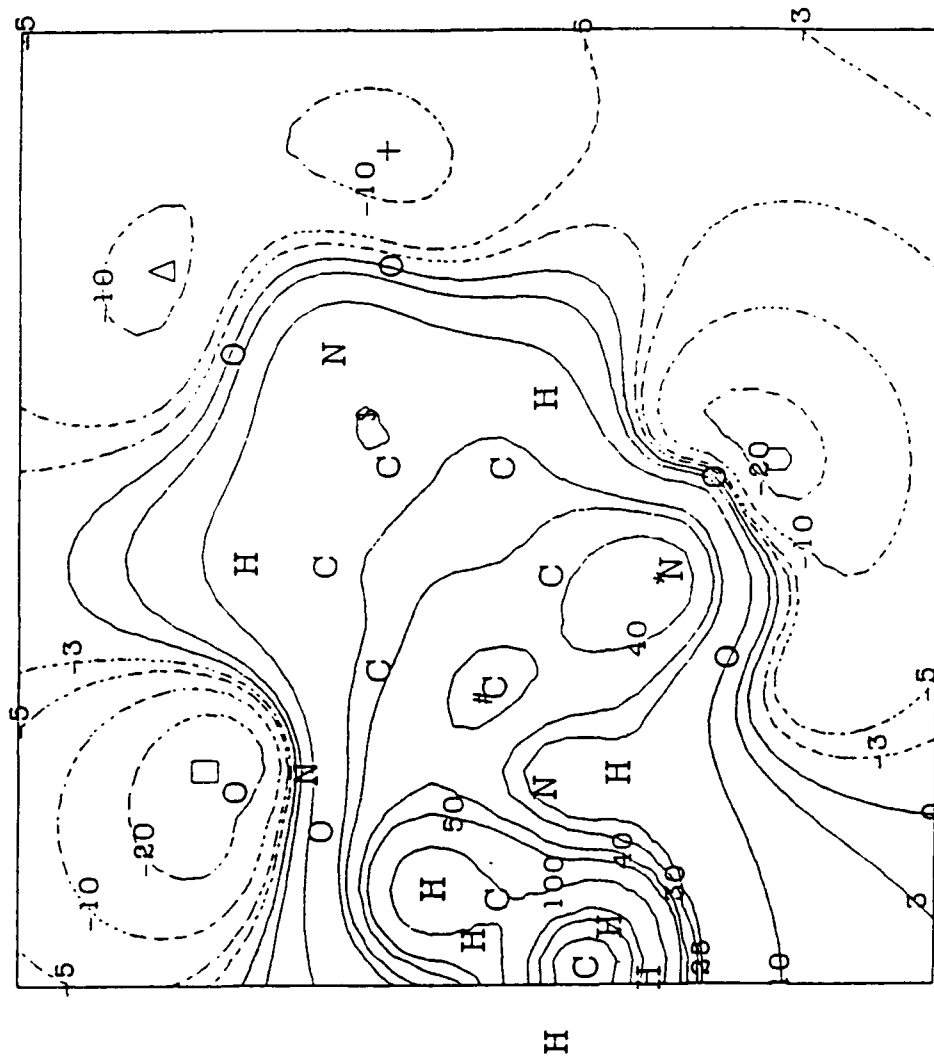
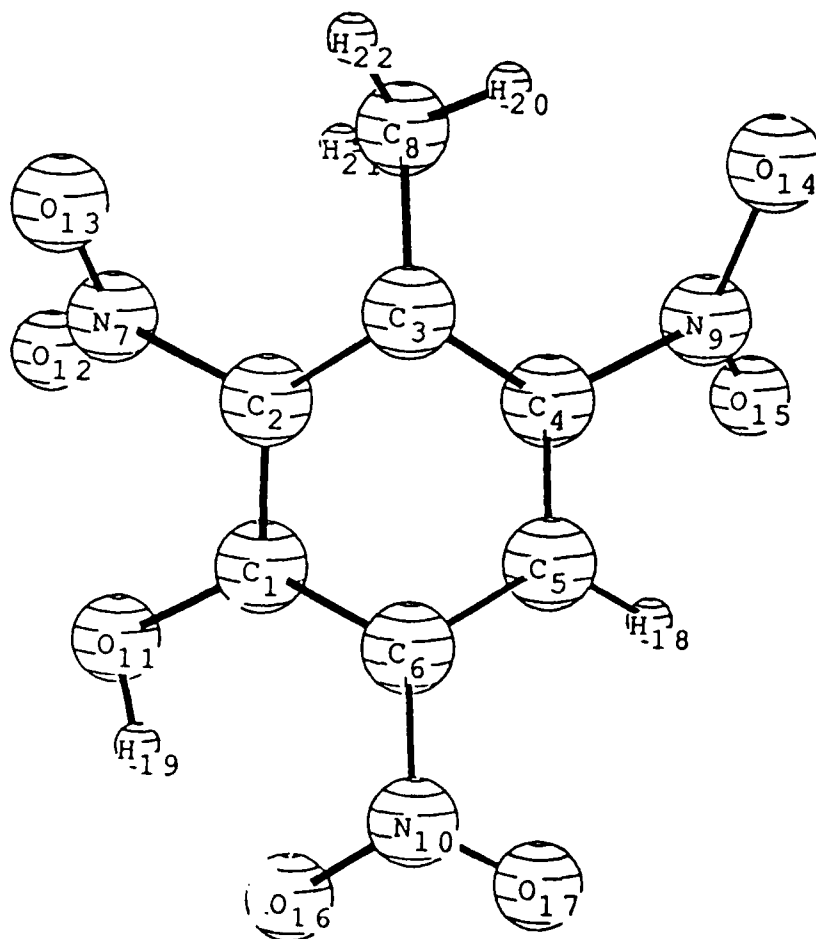


Figure KK-2. Calculated electrostatic potential, in kcal/mole, of N-ethylpicramide, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX LL
3-HYDROXY-2,4,6-TRINITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H21-O14 (2.18 Å), H20-O17 (2.42 Å) and H19-O16 (1.81 Å).

The N7, N9 and N10 nitro groups are rotated by approximately 67°, 42° and 17°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.389000(1)					
3	3	C	2	1.390802(2)	1	123.323(22)			
4	4	C	3	1.380522(3)	2	116.382(23)	1	0.514(42)	0
5	5	C	4	1.363861(4)	3	122.528(24)	2	-1.787(43)	0
6	6	C	5	1.374531(5)	4	120.144(25)	3	-0.410(44)	0
7	7	N	2	1.462911(6)	3	120.070(26)	4	-178.974(45)	0
8	8	C	3	1.519220(7)	4	124.283(27)	5	-177.010(46)	0
9	9	N	4	1.472782(8)	5	116.667(28)	6	-178.754(47)	0
10	10	N	6	1.446781(9)	5	118.634(29)	4	-179.909(48)	0
11	11	O	1	1.342890(10)	2	118.042(30)	3	-179.786(49)	0
12	12	O	7	1.233874(11)	2	118.357(31)	3	111.651(50)	0
13	13	O	7	1.226798(12)	2	117.357(32)	3	-66.311(51)	0
14	14	O	9	1.222853(13)	4	117.759(33)	5	-136.877(52)	0
15	15	O	9	1.230465(14)	4	117.131(34)	5	42.557(53)	0
16	16	O	10	1.236648(15)	6	118.257(35)	5	-164.844(54)	0
17	17	O	10	1.215929(16)	6	117.749(36)	5	19.357(55)	0
18	18	H	5	0.960418(17)	4	119.896(37)	3	179.771(56)	0
19	19	H	11	0.908336(18)	1	104.888(38)	6	1.857(57)	0
20	20	H	8	0.960301(19)	3	109.532(39)	4	-4.787(58)	0
21	21	H	8	0.959471(20)	3	109.528(40)	4	115.323(59)	0
22	22	H	8	0.960519(21)	3	109.413(41)	4	-124.715(60)	0

STOICHIOMETRY C7H5N3O7

SCF DONE: E(RHF) = -950.909243802 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.31314 -0.30340 0.11238 0.14601 0.17979

Estimated ionization potential: 8.26 ev

Total atomic charges:

1	C	0.192800
2	C	0.064872
3	C	0.087716
4	C	0.075010
5	C	-0.046299
6	C	0.052624
7	N	0.165141
8	C	-0.318260
9	N	0.166690
10	N	0.169700
11	O	-0.315936
12	O	-0.179456
13	O	-0.189917
14	O	-0.191096
15	O	-0.190489
16	O	-0.224933
17	O	-0.161141
18	H	0.142403
19	H	0.302241
20	H	0.135493
21	H	0.125994
22	H	0.136842

Dipole moment (Debye):

X=	0.1044	Y=	-0.6909	Z=	-0.1543	Tot=	0.7156
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V-mid: C2-N7: 0.167

C4-N9: 0.174

C6-N10: 0.163

Bond Order: C2-N7: 1.27

C4-N9: 1.24

C6-N10: 1.29

N7-O12: 1.87

N7-O13: 1.91

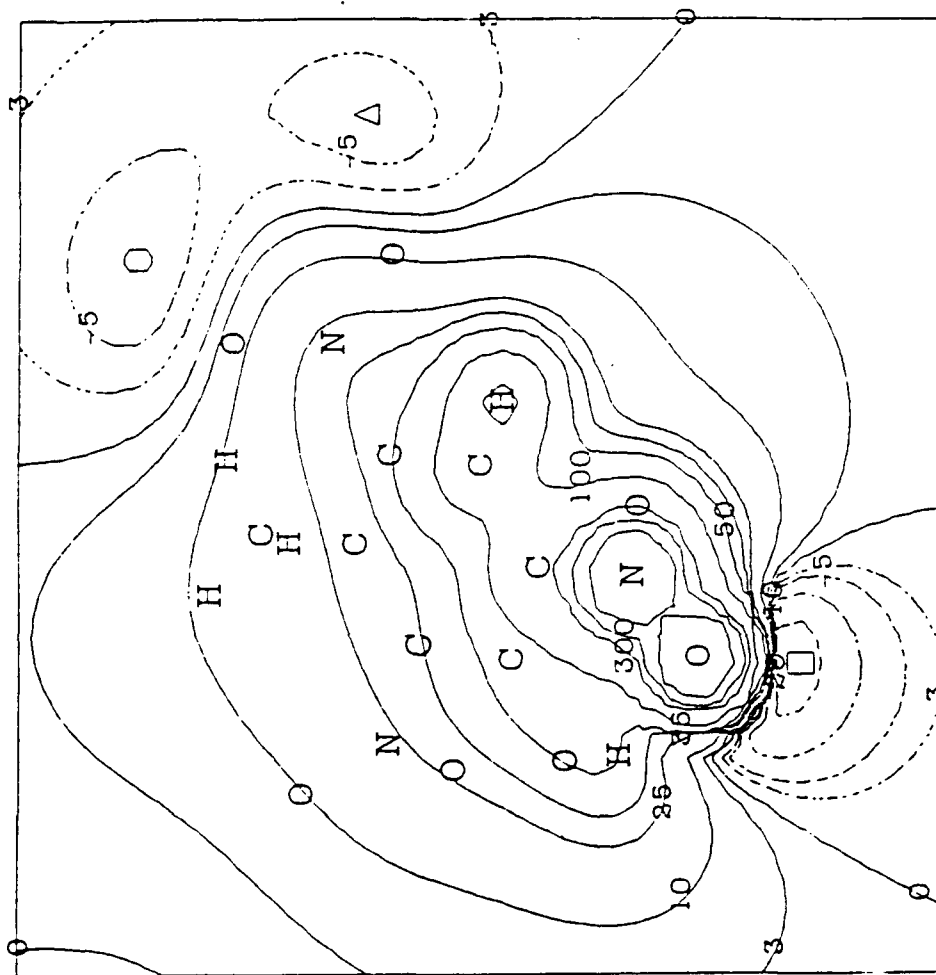
N9-O14: 1.92

N9-O15: 1.89

N10-O16: 1.86

N10-O17: 1.96

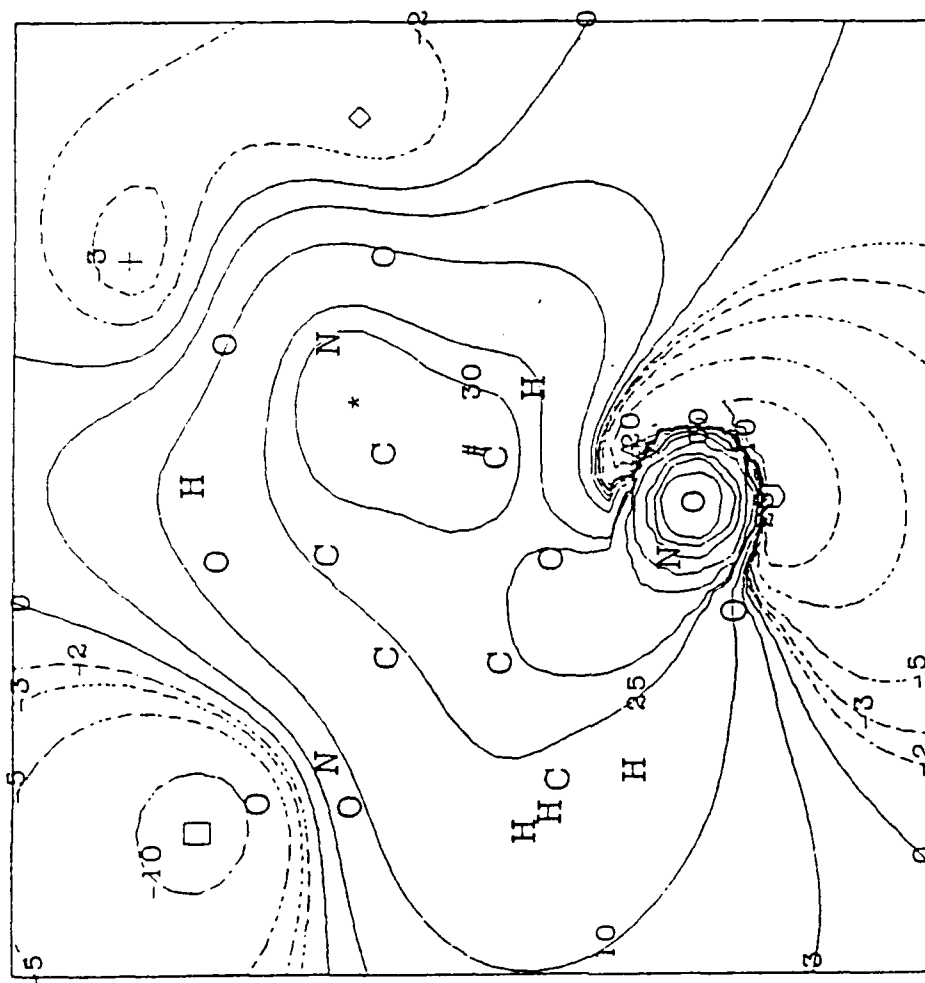
-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
35.0
50.0
100.0
300.0
500.0
1000.0



MINIMA
□ -27.3
○ -6.3
△ -5.9

Figure LL-1. Calculated electrostatic potential, in kcal/mole, of 3-hydroxy-2,4,6-trinitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
-2.0
0.0
3.0
10.0
25.0
30.0
50.0
100.0
300.0
500.0
1000.0



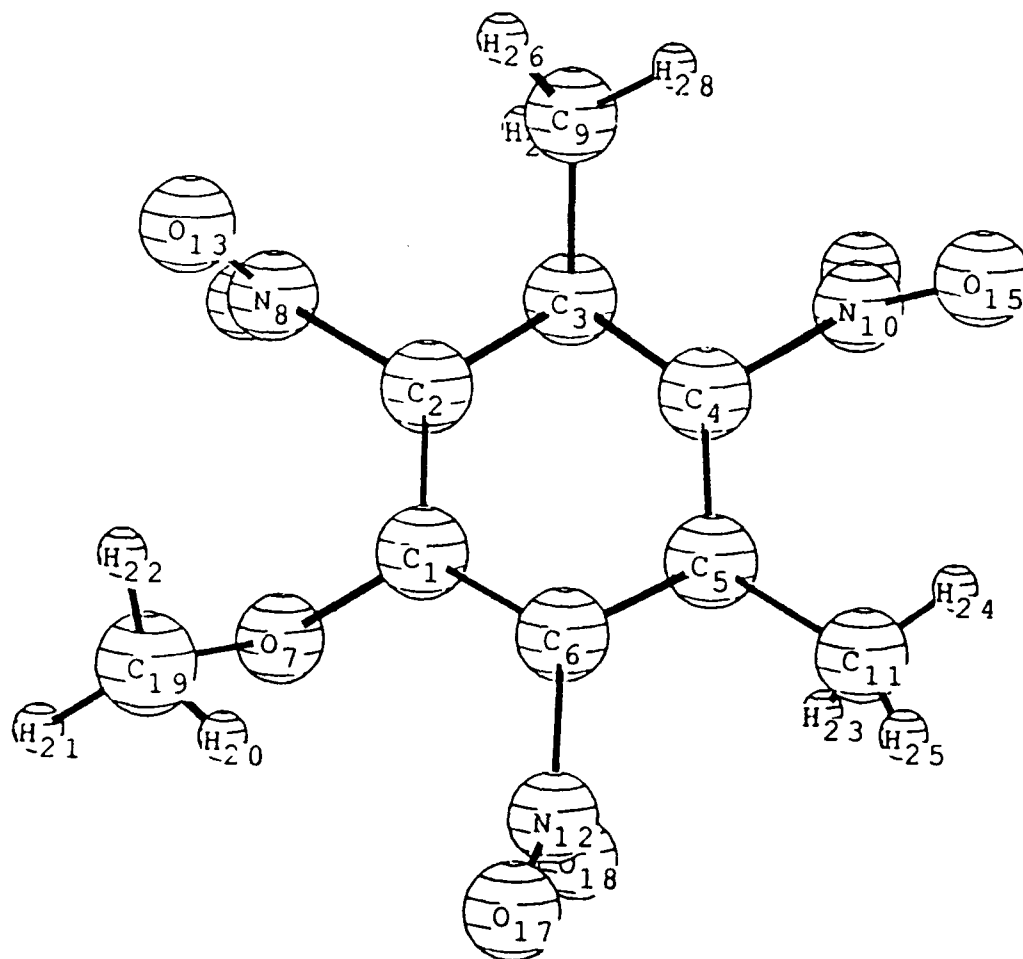
MINIMA	
□	-11.9
○	-40.1
△	-20.6
+	-3.5
◇	-3.0
MAXIMA	
#	+34.4
*	+35.2

Figure LL-2. Calculated electrostatic potential, in kcal/mole, of 3-hydroxy-2,4,6-trinitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX MM
3,5-DIMETHYL-2,4,6-TRINITROANISOLE

All distances between non-bonded hydrogen and oxygen atoms are greater than 2.50 Å.

The N8 nitro group is almost perpendicular to the plane of the benzene ring, while the N10 and N12 nitro groups are both rotated by about 71° and 75°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.358000(1)					
3	3	C	2	1.399318(2)	1	123.009(28)			
4	4	C	3	1.381244(3)	2	113.706(29)	1	-0.330(54)	0
5	5	C	4	1.374427(4)	3	127.264(30)	2	-0.536(55)	0
6	6	C	5	1.380457(5)	4	113.220(31)	3	0.276(56)	0
7	7	O	1	1.381053(6)	2	122.235(32)	3	-173.505(57)	0
8	8	N	2	1.494392(7)	3	118.242(33)	4	-178.931(58)	0
9	9	C	3	1.514005(8)	2	121.506(34)	1	-178.302(59)	0
10	10	N	4	1.474365(9)	5	117.024(35)	6	-178.217(60)	0
11	11	C	5	1.488442(10)	4	123.677(36)	3	-178.810(61)	0
12	12	N	6	1.488545(11)	5	118.590(37)	4	-179.717(62)	0
13	13	O	8	1.195761(12)	2	117.026(38)	3	-86.755(63)	0
14	14	O	8	1.176405(13)	2	117.908(39)	3	94.062(64)	0
15	15	O	10	1.221266(14)	4	119.364(40)	3	109.150(65)	0
16	16	O	10	1.227326(15)	4	118.185(41)	3	-71.237(66)	0
17	17	O	12	1.217146(16)	6	115.962(42)	5	105.055(67)	0
18	18	O	12	1.202357(17)	6	119.010(43)	5	-75.058(68)	0
19	19	C	7	1.410976(18)	1	117.800(44)	2	-78.553(69)	0
20	20	H	19	0.960738(19)	7	98.207(45)	1	-65.863(70)	0
21	21	H	13	0.959901(20)	7	114.169(46)	1	178.350(71)	0
22	22	H	19	0.960835(21)	7	115.396(47)	1	50.294(72)	0
23	23	H	11	0.959732(22)	5	103.633(48)	4	-125.713(73)	0
24	24	H	11	0.960368(23)	5	113.210(49)	4	-7.302(74)	0
25	25	H	11	0.959800(24)	5	111.280(50)	4	116.792(75)	0
26	26	H	9	0.960337(25)	3	106.135(51)	4	-124.700(76)	0
27	27	H	9	0.960321(26)	3	107.094(52)	4	118.482(77)	0
28	28	H	9	0.959719(27)	3	115.051(53)	4	-3.471(78)	0

STOICHIOMETRY C9H9N3O7

SCF DONE: E(RHF) = -1028.63317892 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.34989 -0.32387 -0.31355 -0.30780 0.15926

Estimated ionization energy: 8.34 ev

Total atomic charges:

1		
1	C	0.158660
2	C	0.067981
3	C	0.073648
4	C	0.080800
5	C	0.070937
6	C	0.073606
7	O	-0.241150
8	N	0.199707
9	C	-0.315982
10	N	0.159940
11	C	-0.320361
12	N	0.184359
13	O	-0.212092
14	O	-0.186413
15	O	-0.193336
16	O	-0.194589
17	O	-0.201273
18	O	-0.186486
19	C	-0.179946
20	H	0.123724
21	H	0.131548
22	H	0.117949
23	H	0.134896
24	H	0.129555
25	H	0.132281
26	H	0.130789
27	H	0.132034
28	H	0.129215

Dipole moment (Debye):

X= 0.1680 Y= -0.3563 Z= -1.2833 Tot= 1.3424

Bond Order: C2-N8: 1.18

C4-N10: 1.23

C6-N12: 1.19

N8-O13: 2.06

N8-O14: 2.16

N10-O15: 1.93

N10-O16: 1.91

N11-O17: 1.95

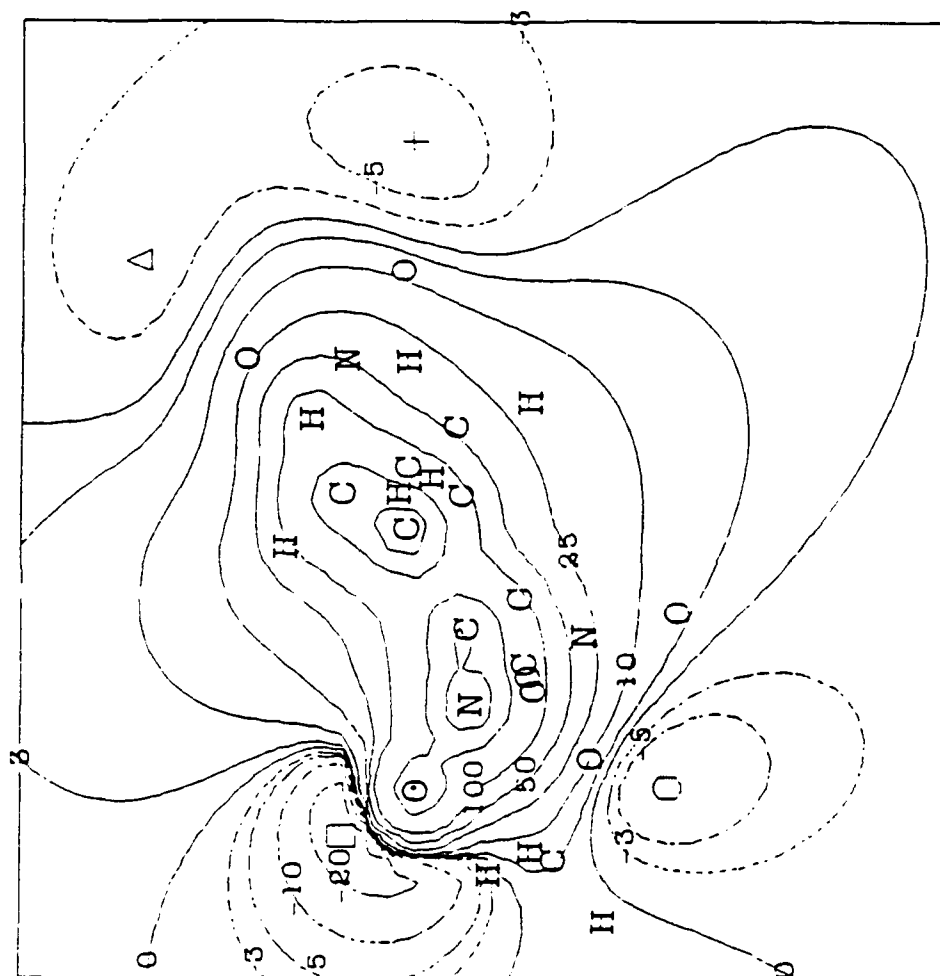
N11-O18: 2.03

V-mid: C2-N8: 0.190

C4-N10: 0.173

C6-N12: 0.184

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0

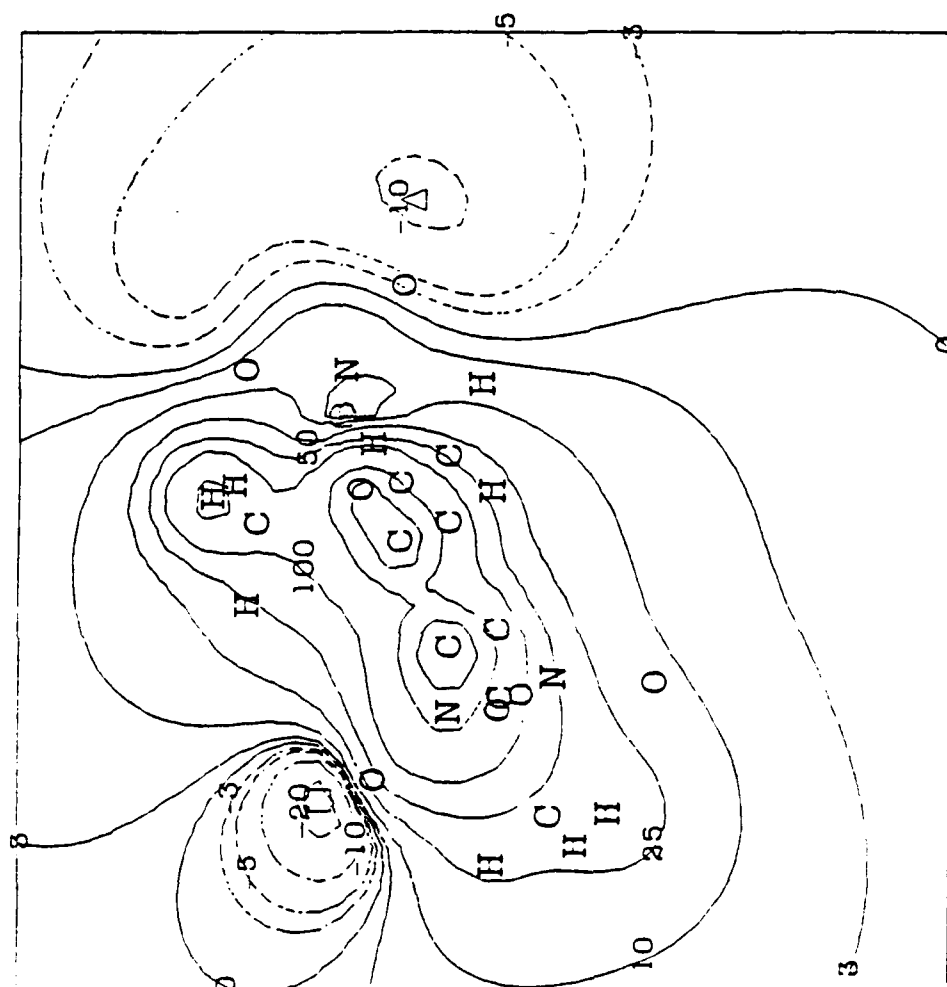


MINIMA

□ -29.4
○ -8.3
△ -4.3
+ -6.4

Figure MM-1. Calculated electrostatic potential, in kcal/mole, of 3,5-dimethyl-2,4,6-trinitroanisole, in the plane 1.75 Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0



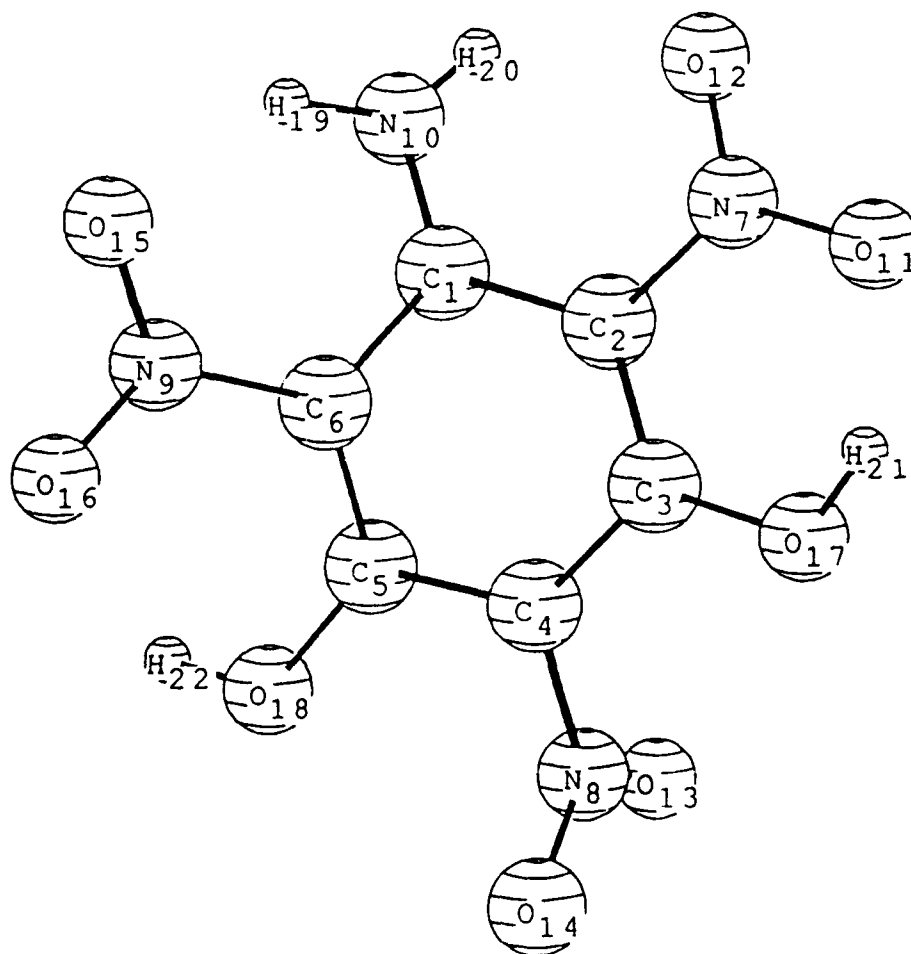
MINIMA
□ -24.7
○ -0.8
△ -10.7

Figure MM-2. Calculated electrostatic potential, in kcal/mole, of 3,5-dimethyl-2,4,6-trinitroanisole, in the plane 1.75Å above the N12 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX NN
2,4,6-TRINITRO-3,5-DIHYDROXYANILINE

The short distances between non-bonded hydrogens and oxygens are H22-O11 (1.68 Å), H20-O12 (1.89 Å), H19-O15 (1.77 Å) and H22-O16 (1.76 Å).

The N7 and N8 nitro groups are rotated out of the mean plane of the benzene ring by about 10° and 57°, respectively, while the N9 nitro group is approximately planar.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C	1	1.433000(1)				
3	3	C	2	1.401292(2)	1	122.054(22)		
4	4	C	3	1.392566(3)	2	119.184(23)	1	3.757(42) 0
5	5	C	4	1.389651(4)	3	121.683(24)	2	-3.991(43) 0
6	6	C	5	1.406808(5)	4	119.432(25)	3	0.574(44) 0
7	7	N	2	1.419691(6)	3	117.928(26)	4	-178.310(45) 0
8	8	N	4	1.451284(7)	3	118.574(27)	2	176.053(46) 0
9	9	N	6	1.429487(8)	5	118.653(28)	4	-176.904(47) 0
10	10	N	1	1.312041(9)	2	122.472(29)	3	178.899(48) 0
11	11	O	7	1.246641(10)	2	119.706(30)	3	-9.464(49) 0
12	12	O	7	1.226492(11)	2	121.595(31)	3	170.181(50) 0
13	13	O	8	1.231708(12)	4	117.251(32)	3	-57.207(51) 0
14	14	O	8	1.200124(13)	4	118.786(33)	3	123.278(52) 0
15	15	O	9	1.231430(14)	6	121.497(34)	5	-179.019(53) 0
16	16	O	9	1.250106(15)	6	118.600(35)	5	1.307(54) 0
17	17	O	3	1.320112(16)	2	124.205(36)	1	-176.920(55) 0
18	18	O	5	1.325487(17)	4	116.486(37)	3	-179.929(56) 0
19	19	H	10	0.959025(18)	1	114.320(38)	2	-171.925(57) 0
20	20	H	10	0.845067(19)	1	114.298(39)	2	3.019(58) 0
21	21	H	17	0.895016(20)	3	106.611(40)	4	-171.735(59) 0
22	22	H	18	0.868143(21)	3	134.968(41)	4	179.432(60) 0

STOICHIOMETRY C5H4N4O8

SCF DONE: E(RHF) = -1041.29860035

Alpha eigenvalues — -0.28233 0.11816 0.13663 0.19340 0.24411

Estimated ionization potential: 7.69 ev

Total atomic charges:

1

1	C	0.237769
2	C	-0.015954
3	C	0.228912
4	C	0.013388
5	C	0.233026
6	C	-0.014067
7	N	0.161212
8	N	0.181797
9	N	0.162517
10	N	-0.530495
11	O	-0.231007
12	O	-0.193961
13	O	-0.202589
14	O	-0.189842
15	O	-0.203892
16	O	-0.223215
17	O	-0.328231
18	O	-0.344611
19	H	0.301574
20	H	0.309182
21	H	0.318936
22	H	0.329549

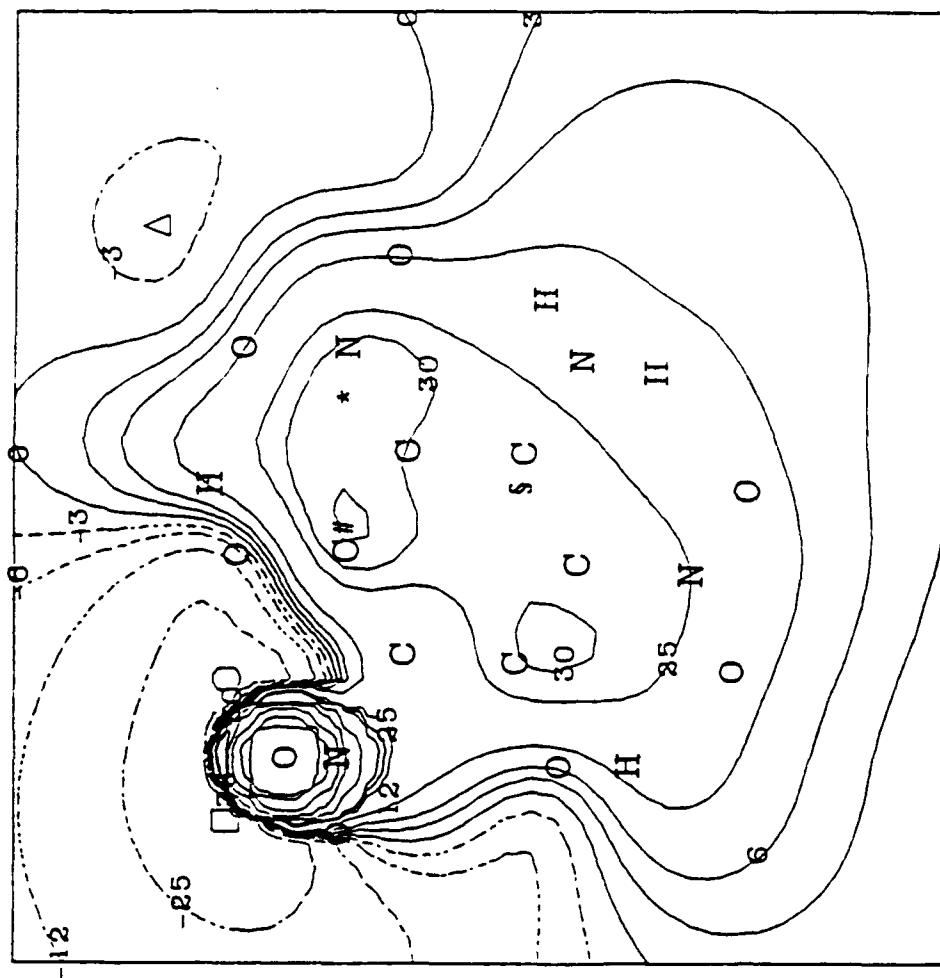
Dipole moment (Debye):

X= -1.5662 Y= -4.1003 Z= -0.3623 Tot= 4.4046

Bond Order: C2-N7: 1.37
 C4-N8: 1.29
 C6-N9: 1.35
 N7-O11: 1.82
 N7-O12: 1.91
 N8-O13: 1.88
 N8-O14: 2.04
 N9-O15: 1.89
 N9-O16: 1.80

V-mid: C2-N7: 0.108
 C4-N8: 0.142
 C6-N9: 0.110

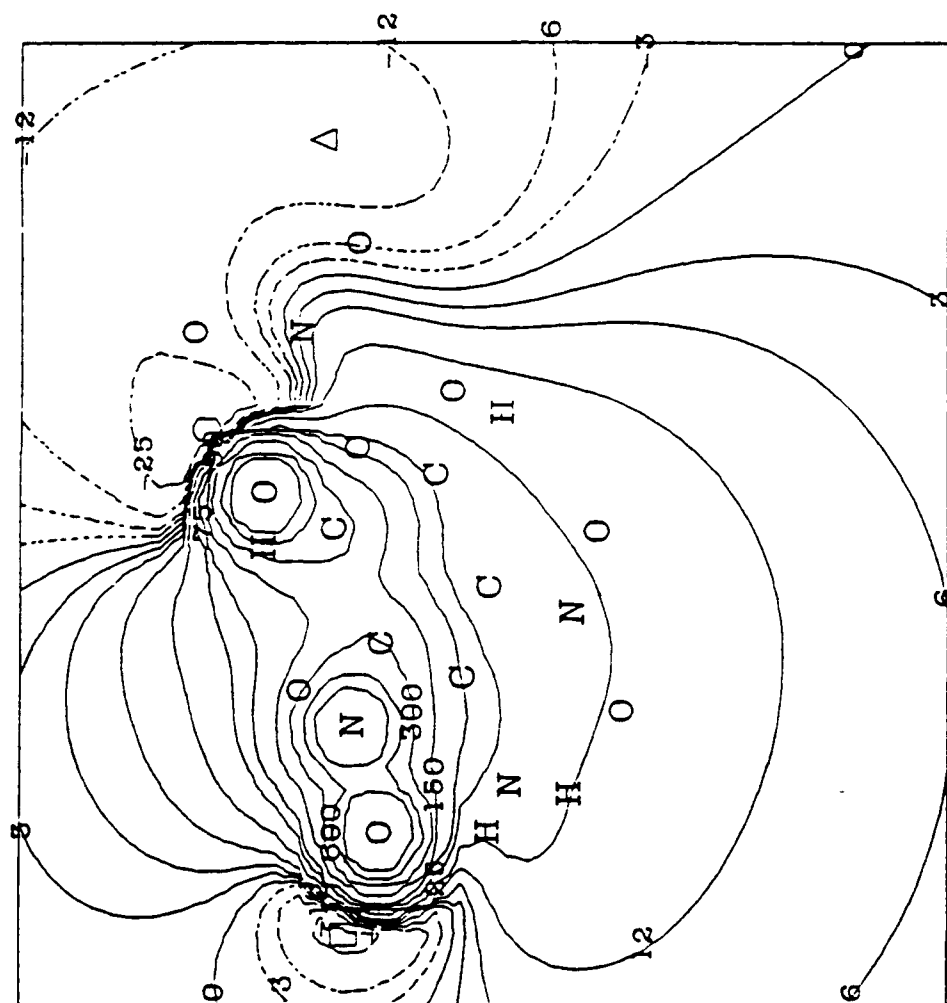
-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
30.0
35.0
75.0
150.0
300.0
600.0
1000.0



MINIMA	
□	-59.1
○	-39.0
△	-3.7
MAXIMA	
*	34.5
#	35.7
\$	30.1

Figure NN-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3,5-dihydroxyaniline, in the plane 1.75Å above the N7 nitro group located in the upper left corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA

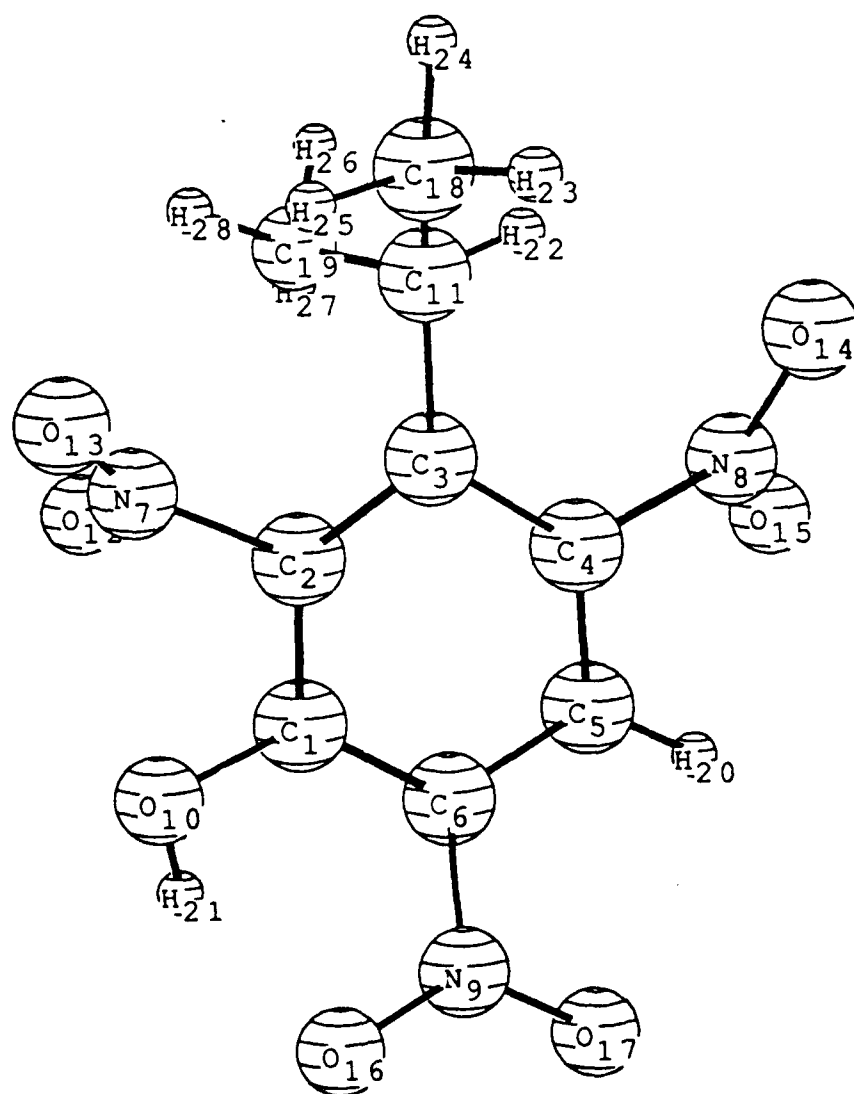
□ -14.6
○ -43.1
△ -16.7

Figure NN-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3,5-dihydroxyaniline, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX OO
1-HYDROXY-3-ISOPROPYL-2,4,6-TRINITROBENZENE

The short distances between non-bonded hydrogens and oxygens are H21-O16 (1.89 Å), H20-O17 (2.46 Å) and H22-O14 (2.51 Å).

The N7 nitro group is rotated out of the plane by about 80° and the N8 nitro group is rotated by about 55°, while the N9 nitro group is essentially planar.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.388000(1)				
3	3	C	2	1.387669(2)	1	125.921(28)		
4	4	C	3	1.405766(3)	2	112.354(29)	1	4.635(54)
5	5	C	4	1.358591(4)	3	125.030(30)	2	-1.979(55)
6	6	C	5	1.383269(5)	4	119.124(31)	3	-1.896(56)
7	7	N	2	1.485639(6)	3	121.698(32)	4	-178.485(57)
8	8	N	4	1.480245(7)	5	114.723(33)	6	177.753(58)
9	9	N	6	1.457886(8)	5	118.408(34)	4	-176.960(59)
10	10	O	1	1.338471(9)	2	116.876(35)	3	175.275(60)
11	11	C	3	1.516254(10)	2	124.647(36)	1	-175.831(61)
12	12	O	7	1.213447(11)	2	117.125(37)	3	102.887(62)
13	13	O	7	1.207865(12)	2	117.419(38)	3	-79.577(63)
14	14	O	8	1.210975(13)	4	118.600(39)	3	55.976(64)
15	15	O	8	1.215999(14)	4	117.321(40)	3	-126.918(65)
16	16	O	9	1.235425(15)	6	117.244(41)	5	176.488(66)
17	17	O	9	1.202063(16)	6	119.247(42)	5	-3.129(67)
18	18	C	11	1.544227(17)	3	110.25(43)	2	84.399(68)
19	19	C	11	1.531956(18)	3	115.001(44)	2	-42.333(69)
20	20	H	5	0.978625(19)	4	118.069(45)	3	175.972(70)
21	21	H	10	0.793650(20)	1	104.145(46)	2	179.251(71)
22	22	H	11	0.960347(21)	3	108.571(47)	4	21.738(72)
23	23	H	18	0.959416(22)	11	111.938(48)	3	53.237(73)
24	24	H	18	0.960172(23)	11	108.037(49)	3	173.942(74)
25	25	H	18	0.960073(24)	11	108.334(50)	3	-67.580(75)
26	26	H	19	0.960102(25)	11	107.446(51)	3	-166.508(76)
27	27	H	19	0.960241(26)	11	110.618(52)	3	-47.132(77)
28	28	H	19	0.960081(27)	11	110.504(53)	3	74.208(78)

STOICHIOMETRY C9H9N3O7

CF DONE: E(RHF) = -1028.63602740 A.U. AFTER 22 CYCLES

Alpha eigenvalues — -0.33832 -0.33330 -0.31251 -0.30798 0.11642

Estimated ionization potential: 8.39 ev

Total atomic charges:

1
 1 C 0.192208
 2 C 0.068542
 3 C 0.064438
 4 C 0.079993
 5 C -0.049027
 6 C 0.052344
 7 N 0.185430
 8 N 0.172991
 9 N 0.175261
 10 O -0.379352
 11 C -0.034239
 12 O -0.190142
 13 O -0.194737
 14 O -0.196555
 15 O -0.197313
 16 O -0.230134
 17 O -0.167135
 18 C -0.299204
 19 C -0.303012
 20 H 0.140570
 21 H 0.350573
 22 H 0.100882
 23 H 0.111085
 24 H 0.109257
 25 H 0.111096
 26 H 0.110161
 27 H 0.105843
 28 H 0.108075

Dipole moment (Debye):

X= -0.6133 Y= 0.5527 Z= -0.0293 Tot= 0.8261

V-mid: C2-N7: 0.182

C4-N8: 0.181

C6-N9: 0.165

Bond Order: C2-N7: 1.20

C4-N8: 1.21

C6-N9: 1.27

N7-O12: 1.97

N7-O13: 2.00

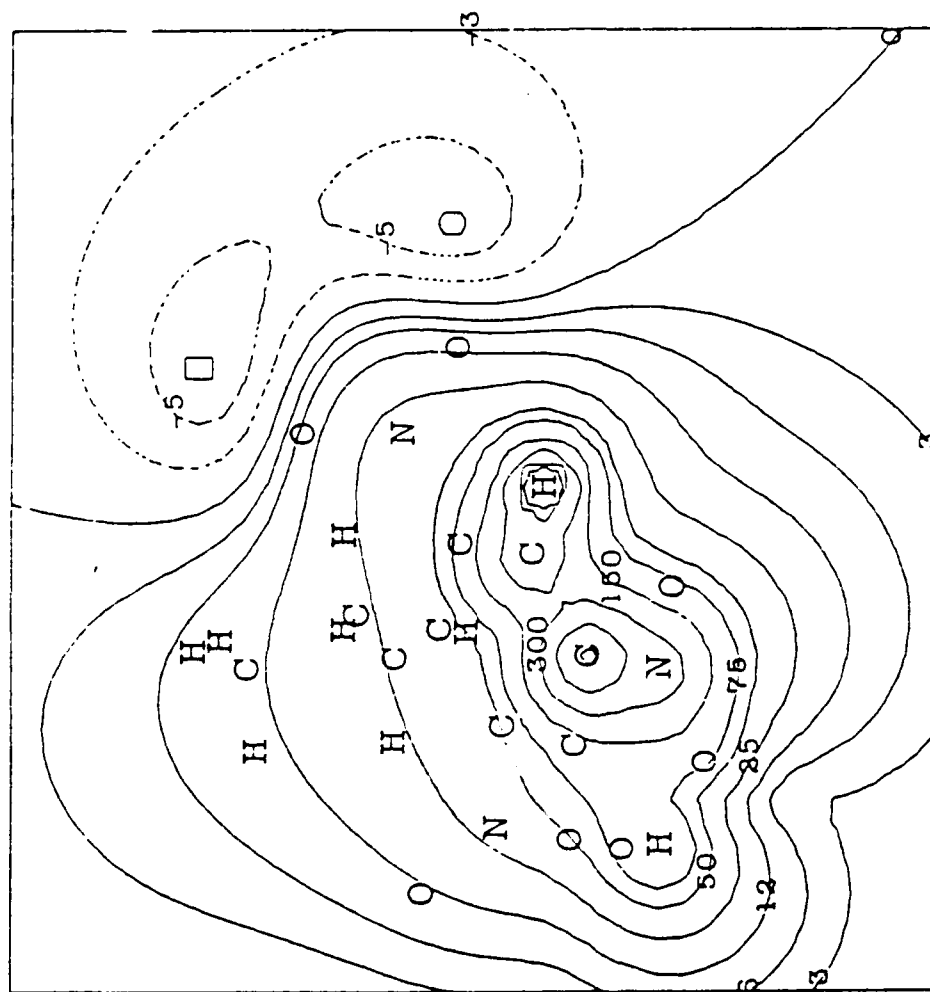
N6-O14: 1.98

N8-O15: 1.96

N9-O16: 1.87

N9-O17: 2.03

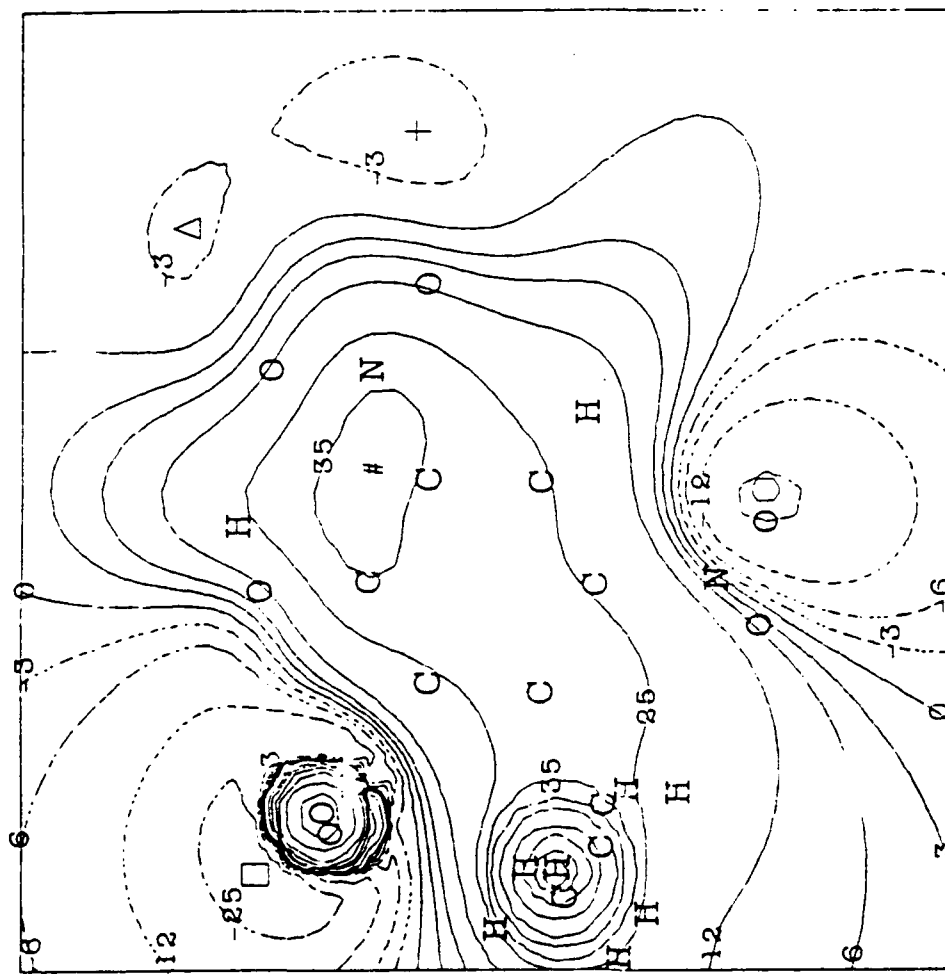
-5.0
-3.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA

□ -6.0
○ -6.0

Figure OO-1. Calculated electrostatic potential, in kcal/mole, of 1-hydroxy-3-isopropyl-2,4,6-trinitrobenzene, in the plane 1.75Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.



\square	-41.3
\bigcirc	-27.2
\triangle	-3.3
$+$	-3.8

MAXIMA

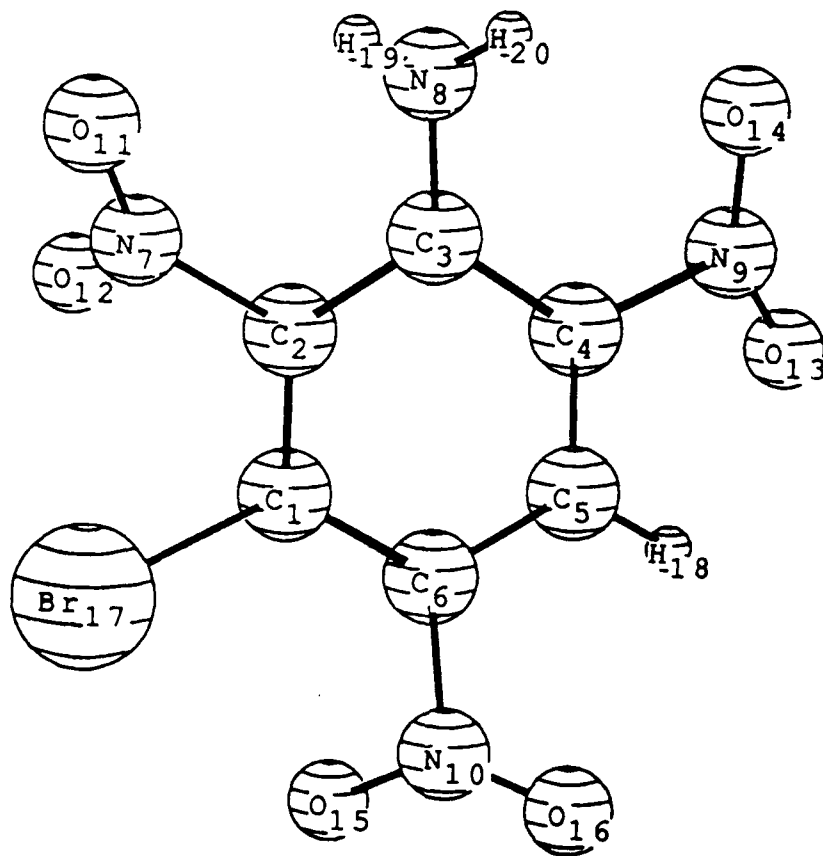
+37.7

Figure OO-2. Calculated electrostatic potential, in kcal/mole, of 1-hydroxy-3-isopropyl-2,4,6-trinitrobenzene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX PP
3-BROMO-2,4,6-TRINITROANILINE

The short distances between non-bonded hydrogens and oxygens are H18-O13 (2.36 Å), H20-O14 (2.08 Å) and H19-O11 (2.43 Å).

The N7, N9 and N10 nitro groups are rotated by approximately 65°, 18°, and 28°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.372000(1)					
3	3	C	2	1.424368(2)	1	124.674(20)			
4	4	C	3	1.405510(3)	2	113.461(21)	1	7.533(38)	0
5	5	C	4	1.366465(4)	3	122.424(22)	2	-7.636(39)	0
6	6	C	5	1.369559(5)	4	120.969(23)	3	3.834(40)	0
7	7	N	2	1.477968(6)	3	116.350(24)	4	-173.750(41)	0
8	8	N	3	1.346803(7)	2	121.284(25)	1	-174.924(42)	0
9	9	N	4	1.454183(8)	5	116.924(26)	6	-176.688(43)	0
10	10	N	6	1.473321(9)	5	116.102(27)	4	-178.449(44)	0
11	11	O	7	1.204854(10)	2	117.583(28)	1	115.162(45)	0
12	12	O	7	1.209212(11)	2	117.654(29)	1	-66.867(46)	0
13	13	O	9	1.212505(12)	4	117.722(30)	5	18.395(47)	0
14	14	O	9	1.216614(13)	4	119.350(31)	5	-162.578(48)	0
15	15	O	10	1.224901(14)	6	118.331(32)	5	-149.334(49)	0
16	16	O	10	1.218068(15)	6	117.218(33)	5	27.587(50)	0
17	17	Br	1	1.878236(16)	2	118.492(34)	3	172.183(51)	0
18	18	H	5	0.922272(17)	4	119.131(35)	3	-177.37(52)	0
19	19	H	8	0.677642(18)	3	118.041(36)	2	0.621(53)	0
20	20	H	8	0.732741(19)	3	115.600(37)	2	174.196(54)	0

STOICHIOMETRY C6H3BrN4O6

SCF DONE: E(RHF) = -3450.13321750 A.U. AFTER 27 CYCLES

Alpha eigenvalues — -0.33612 -0.32384 -0.32244 -0.31168 0.11827

Estimated ionization potential: 8.49 ev

Total atomic charges:

1
 1 C -0.017044
 2 C 0.069692
 3 C 0.241481
 4 C 0.072043
 5 C -0.058216
 6 C 0.081735
 7 N 0.176424
 8 N -0.761201
 9 N 0.176836
 10 N 0.171671
 11 O -0.195344
 12 O -0.183900
 13 O -0.186679
 14 O -0.211035
 15 O -0.186558
 16 O -0.191160
 17 Br 0.112995
 18 H 0.152885
 19 H 0.367661
 20 H 0.367844

Dipole moment (Debye):

X= 0.8162 Y= -1.3947 Z= -0.5005 Tot= 1.6917

V-mid: C2-N7: 0.176

C4-N8: 0.181

C6-N9: 0.183

Bond Order: C2-N7: 1.22

C4-N8: 1.28

C6-N9: 1.23

N7-O11: 2.01

N7-O12: 1.99

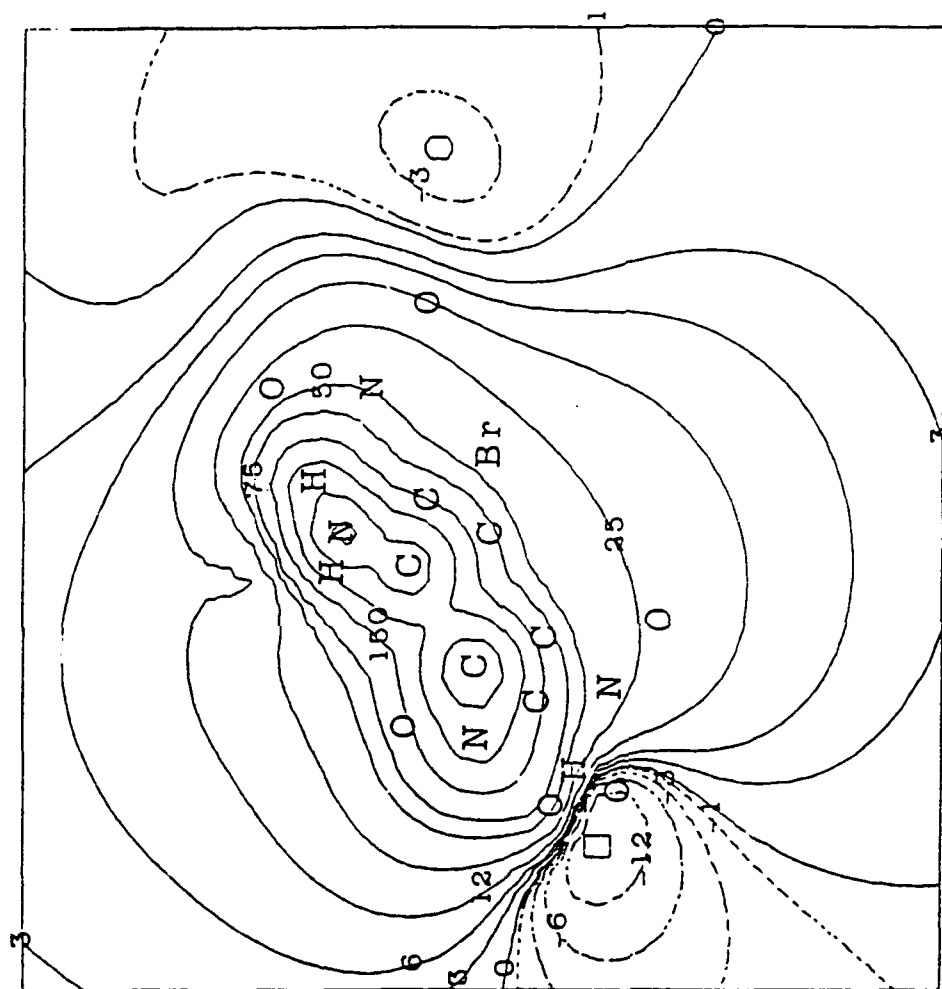
N8-O13: 1.97

N9-O14: 1.95

N10-O15: 1.91

N10-O16: 1.95

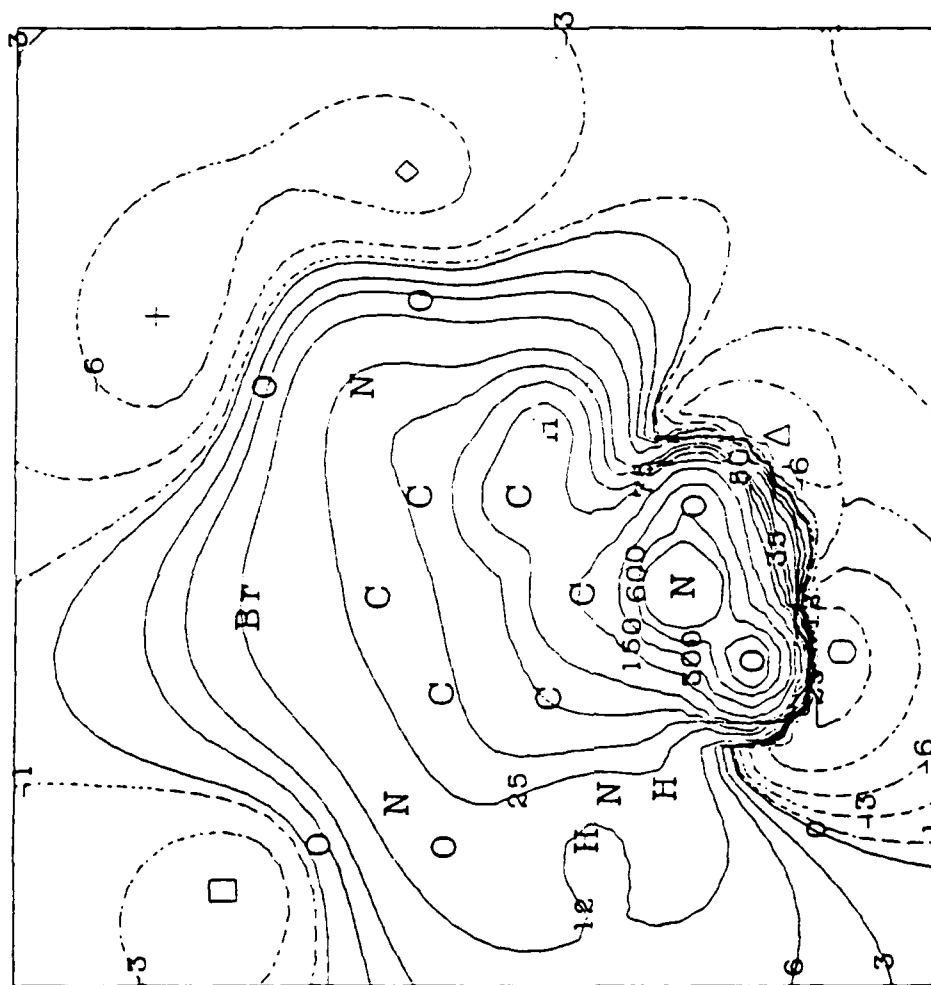
-12.0
-6.0
-3.0
-1.0
0.0
3.0
6.0
12.0
25.0
50.0
75.0
150.0
300.0
600.0
1000.0



MINIMA
□ -21.7
○ -3.6

Figure PP-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N7 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-25.0
-12.0
-6.0
-3.0
-1.0
0.0
3.0
6.0
12.0
25.0
35.0
50.0
75.0
150.0
300.0
600.0
1000.0



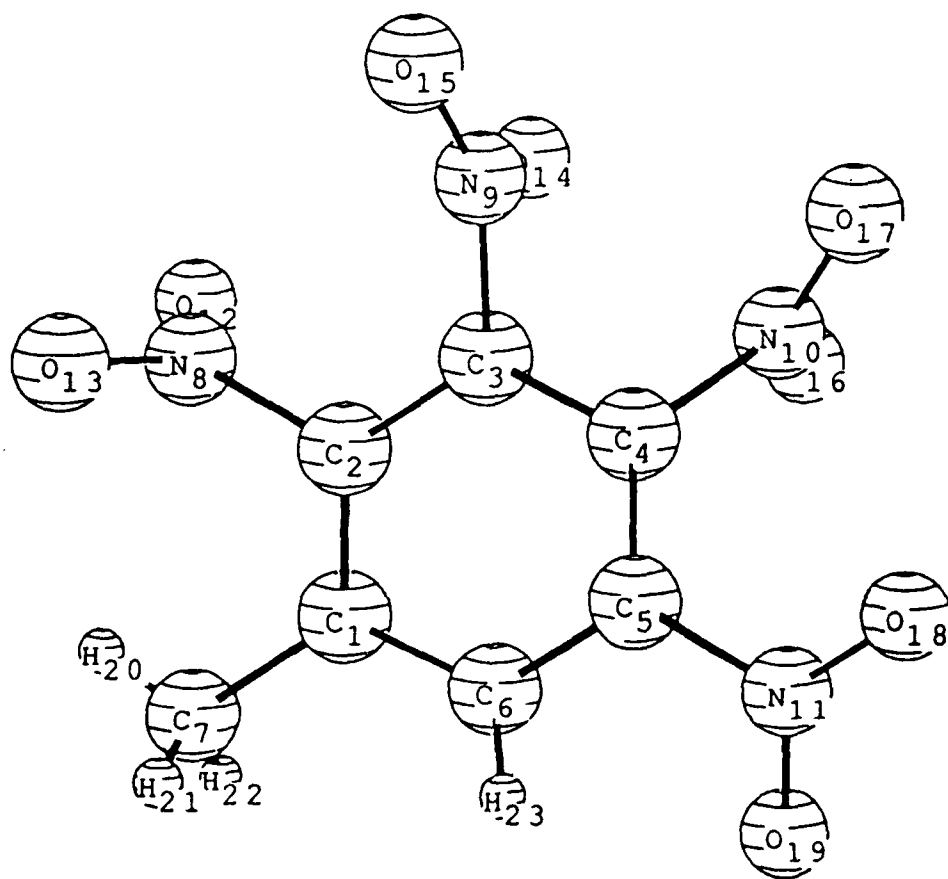
MINIMA
□ -4.6
○ -37.7
△ -8.5
+ -7.8
◇ -7.1

Figure PP-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroaniline, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX QQ
2,3,4,5-TETRANITROTOLUENE

The short distances between a non-bonded hydrogen and oxygen are H20-O13 (2.41 Å) and H23-O19 (2.37 Å).

The N8, N9, N10 and N11 nitro groups are rotated out of the mean plane of the benzene ring by about 52°, 57°, 70° and 17°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)									
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z	J
1	1	C							
2	2	C	1	1.386000(1)					
3	3	C	2	1.389914(2)	1	122.670(23)			
4	4	C	3	1.386169(3)	2	120.086(24)	1	-0.531(44)	0
5	5	C	4	1.388959(4)	3	117.977(25)	2	-1.559(45)	0
6	6	C	5	1.372667(5)	4	121.030(26)	3	1.832(46)	0
7	7	C	1	1.499494(6)	2	123.471(27)	3	-175.907(47)	0
8	8	N	2	1.476841(7)	3	117.175(28)	4	-175.195(48)	0
9	9	N	3	1.469061(8)	4	119.387(29)	5	177.288(49)	0
10	10	N	4	1.472367(9)	5	123.988(30)	6	-177.134(50)	0
11	11	N	5	1.476757(10)	4	121.230(31)	3	-176.260(51)	0
12	12	O	8	1.220058(11)	2	116.667(32)	3	52.701(52)	0
13	13	O	8	1.220096(12)	2	117.668(33)	3	-127.694(53)	0
14	14	O	9	1.215757(13)	3	117.034(34)	4	56.748(54)	0
15	15	O	9	1.213007(14)	3	116.934(35)	4	-121.648(55)	0
16	16	O	10	1.203945(15)	4	117.557(36)	5	70.280(56)	0
7	17	O	10	1.215721(16)	4	116.552(37)	5	-111.938(57)	0
18	18	O	11	1.218650(17)	5	116.738(38)	6	-161.648(58)	0
19	19	O	11	1.207000(18)	5	118.200(39)	6	16.600(59)	0
20	20	H	7	0.960042(19)	1	111.415(40)	2	10.127(60)	0
21	21	H	7	0.959226(20)	1	108.817(41)	2	-110.677(61)	0
22	22	H	7	0.960381(21)	1	108.144(42)	2	130.423(62)	0
23	23	H	6	0.899000(22)	5	117.121(43)	4	178.993(63)	0

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.84669927 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.33526 -0.33225 -0.32882 -0.32413 0.09313

Estimated ionization potential: 8.83 ev

Total atomic charges:

1
 1 C 0.086743
 2 C 0.104312
 3 C 0.117021
 4 C 0.111062
 5 C 0.120064
 6 C -0.090093
 7 C -0.314426
 8 N 0.173332
 9 N 0.182791
 10 N 0.194078
 11 N 0.183363
 12 O -0.180278
 13 O -0.174823
 14 O -0.168316
 15 O -0.170357
 16 O -0.163796
 17 O -0.177225
 18 O -0.180773
 19 O -0.180193
 20 H 0.129860
 21 H 0.132950
 22 H 0.127817
 23 H 0.136886

Dipole moment (Debye):

X= -1.1539 Y= 6.0775 Z= 0.1396 Tot= 6.1877

V-mid: C2-N8: 0.198

C3-N9: 0.216

C4-N10: 0.220

C5-N11: 0.217

Bond Order: C2-N8: 1.22

C3-N9: 1.24

C4-N10: 1.23

C5-N11: 1.22

N8-O12: 1.94

N8-O13: 1.94

N9-O14: 1.96

N9-O15: 1.97

N10-O16: 2.02

N10-O17: 1.96

N11-O18: 1.94

N11-O19: 2.00

-20.0
-15.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0

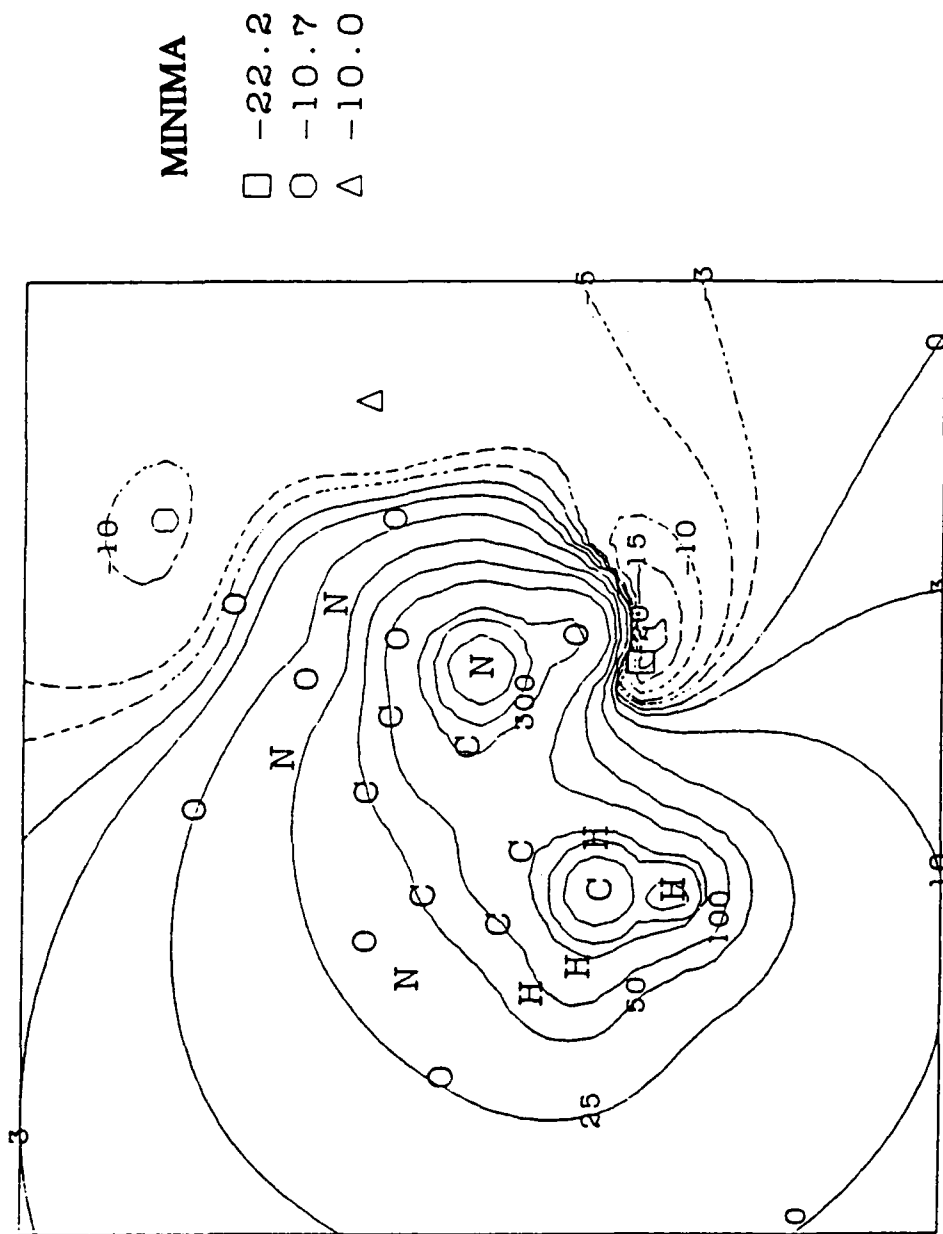
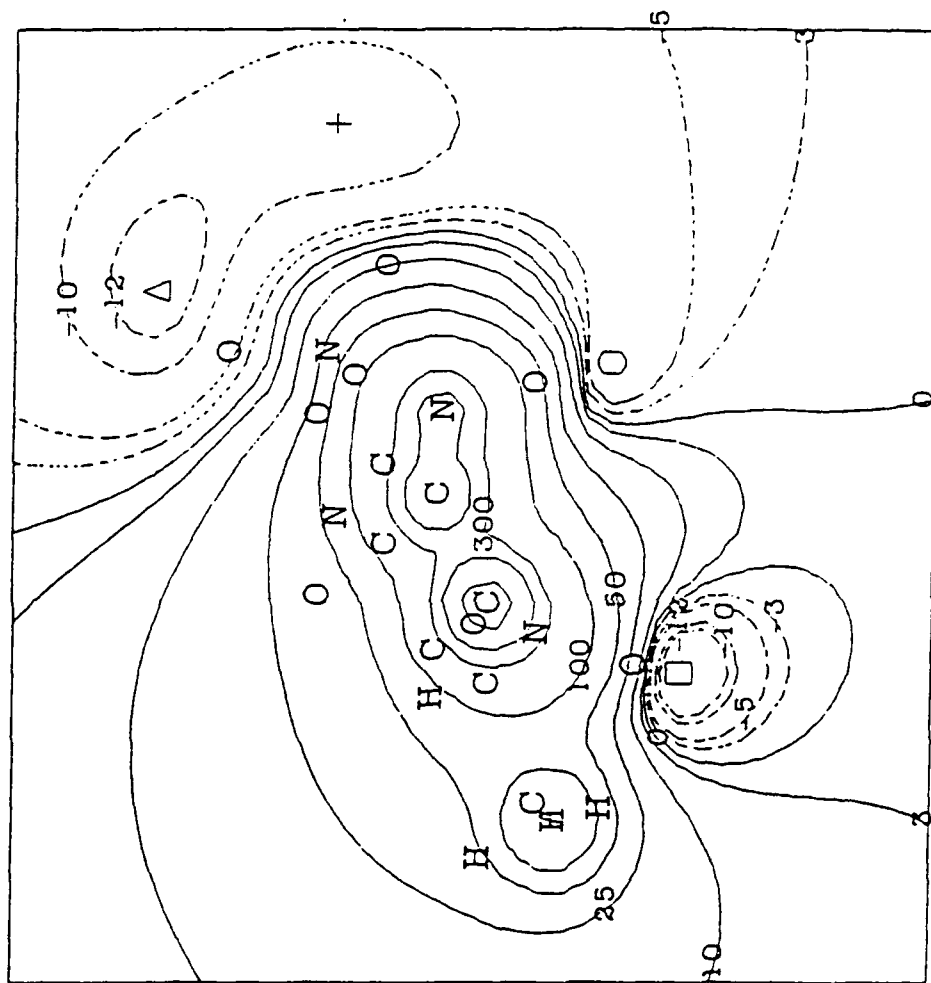


Figure QQ-1. Calculated electrostatic potential, in kcal/mole, of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-12.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA

□ -20.7
○ -9.0
△ -13.1
+ -11.9

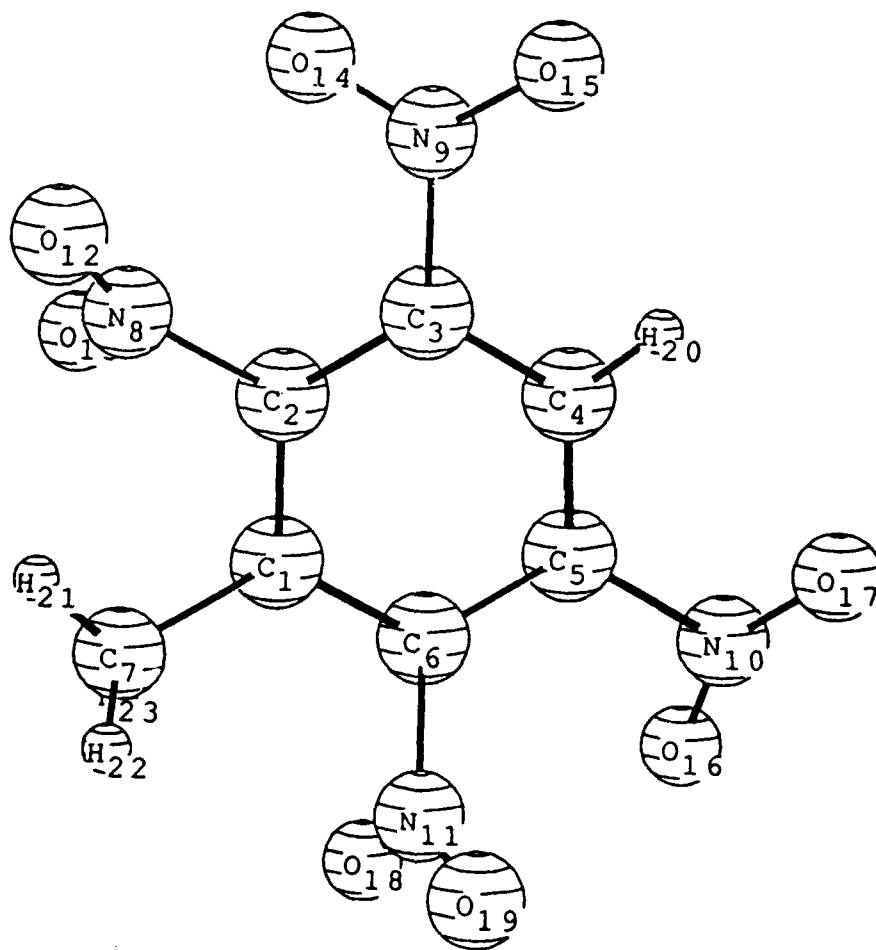
Figure QQ-2. Calculated electrostatic potential, in kcal/mole, of 2,3,4,5-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX RR

2,3,5,6-TETRANITROTOLUENE

The short non-bonded oxygen hydrogen distance is H20-O15 (2.36 Å).

The N8, N9, N10, and N11 nitro groups are both rotated by approximately 80°, 15°, 32° and 70°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.400000(1)				
3	3	C	2	1.381443(2)	1	121.398(23)		
4	4	C	3	1.373904(3)	2	120.468(24)	1	2.503(44)
5	5	C	4	1.345872(4)	3	119.936(25)	2	-1.597(45)
6	6	C	5	1.393176(5)	4	119.747(26)	3	-0.917(46)
7	7	C	1	1.515595(6)	2	122.117(27)	3	176.670(47)
8	8	N	2	1.466849(7)	3	122.671(28)	4	-178.772(48)
9	9	N	3	1.461898(8)	4	118.559(29)	5	178.408(49)
10	10	N	5	1.470476(9)	4	119.310(30)	3	-179.517(50)
11	11	N	6	1.483591(10)	5	120.979(31)	4	-173.462(51)
12	12	O	8	1.206716(11)	2	117.742(32)	3	-80.970(52)
13	13	O	2	1.229347(12)	2	116.005(33)	3	102.264(53)
14	14	O	9	1.212008(13)	3	118.626(34)	2	-14.555(54)
15	15	O	9	1.218880(14)	3	118.289(35)	2	164.893(55)
16	16	O	10	1.206272(15)	5	117.139(36)	4	-146.656(56)
17	17	O	10	1.190841(16)	5	117.324(37)	4	30.116(57)
18	18	O	11	1.213804(17)	6	117.883(38)	5	-111.442(58)
19	19	O	11	1.216086(18)	6	115.667(39)	5	72.188(59)
20	20	H	4	0.921252(19)	3	115.638(40)	2	-178.564(60)
21	21	H	7	0.959480(20)	1	107.768(41)	2	-7.718(61)
22	22	H	7	0.960219(21)	1	110.985(42)	2	-127.608(62)
23	23	H	7	0.960329(22)	1	109.673(43)	2	111.411(63)

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.85136659 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.33701 -0.33399 -0.33046 -0.32624 0.08686

ESTIMATED IONIZATION POTENTIAL: 8.88 eV

Total atomic charges:

1	C	0.070719
2	C	0.112801
3	C	0.118821
4	C	-0.079733
5	C	0.116625
6	C	0.110954
7	C	-0.314021
8	N	0.181539
9	N	0.177002
10	N	0.195248
11	N	0.183539
12	O	-0.170716
13	O	-0.179174
14	O	-0.178712
15	O	-0.180401
16	O	-0.188083
17	O	-0.177373
18	O	-0.172127
19	O	-0.181751
20	H	0.155393
21	H	0.127928
22	H	0.131383
23	H	0.140140

Dipole moment (Debye):

X= 0.0105 Y= -0.9166 Z= -0.1413 Tot= 0.9275

V-mid: C2-N8: 0.212

C3-N9: 0.214

C5-N10: 0.225

C6-N11: 0.211

Bond order: C2-N8: 1.24

C3-N9: 1.27

C5-N10: 1.24

C6-N11: 1.21

N8-O12: 2.00

N8-O13: 1.90

N9-O14: 1.98

N9-O15: 1.94

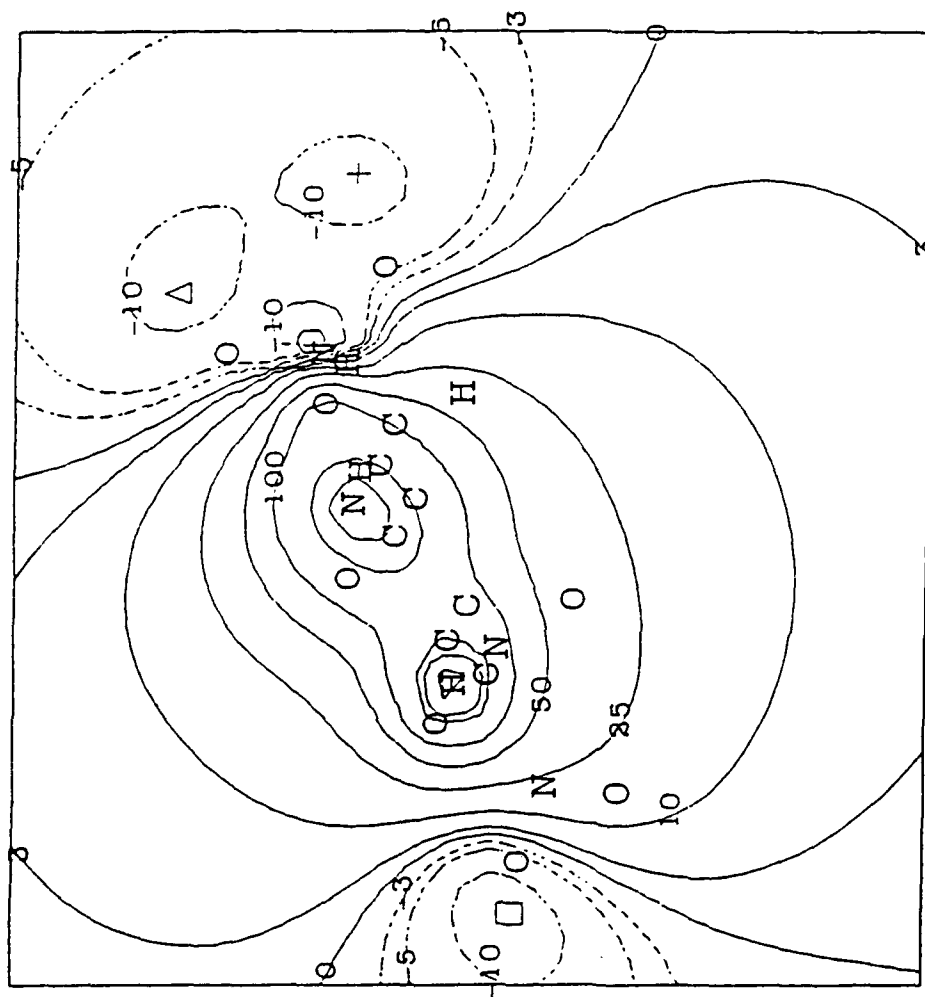
N10-O16: 2.01

N10-O17: 2.04

N11-O18: 1.97

N11-O19: 1.96

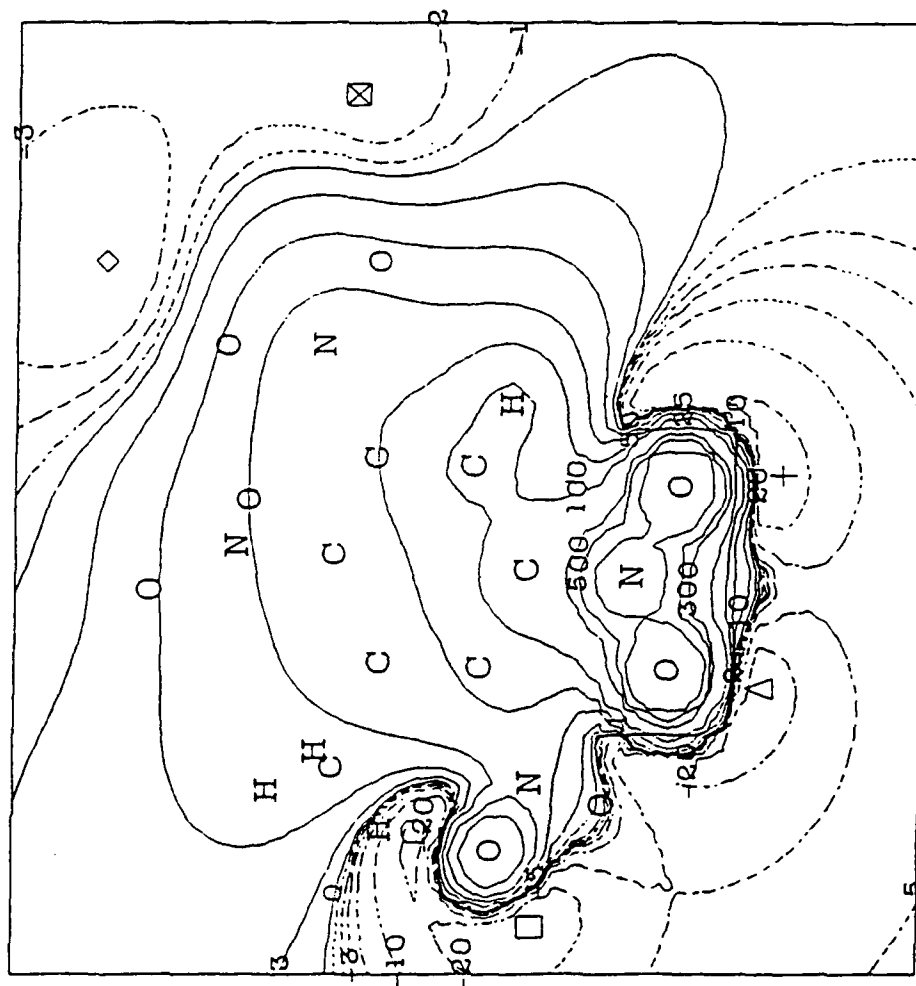
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA
□ -13.0
○ -12.7
△ -11.3
+ -11.0

Figure RR-1. Calculated electrostatic potential, in kcal/mole, of 2,3,5,6-tetranitrotoluene, in the plane 1.75 Å above the N8 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
-2.0
-1.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA

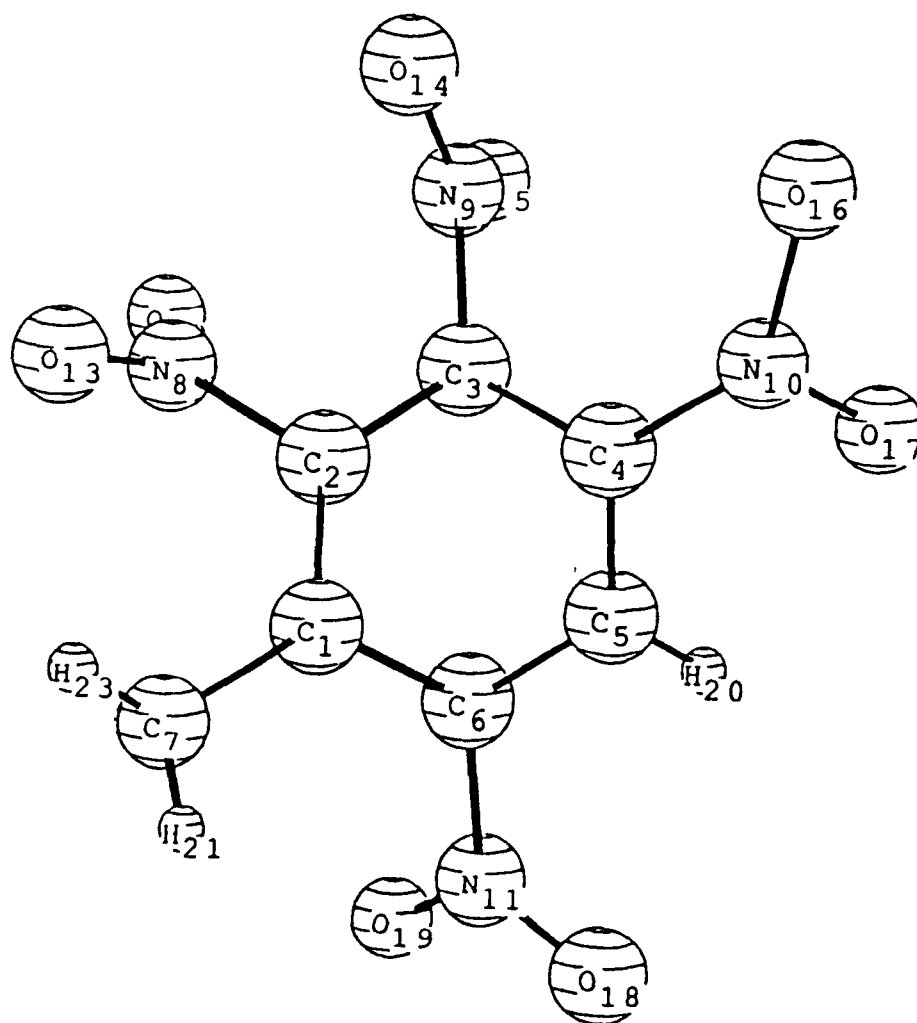
□ -33.4
○ -24.7
△ -30.1
+ -28.6
◇ -4.3
⊠ -2.8

Figure RR-2. Calculated electrostatic potential, in kcal/mole, of 2,3,5,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX SS
2,3,4,6-TETRANITROTOLUENE

The short distances between non-bonded hydrogens and oxygens are H20-O17 (2.47 Å), H21-O19 (2.44 Å) and H23-O13 (2.36 Å)

The N8, N9, N10 and N11 nitro groups are rotated out of the mean plane of the benzene ring by approximately 62°, 68°, 27° and 47°, respectively.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.389000(1)				
3	3	C	2	1.375172(2)	1	123.720(23)		
4	4	C	3	1.383634(3)	2	119.370(24)	1	-1.863(44)
5	5	C	4	1.371733(4)	3	119.918(25)	2	2.169(45)
6	6	C	5	1.373445(5)	4	118.712(26)	3	0.223(46)
7	7	C	1	1.492121(6)	2	123.285(27)	3	178.926(47)
8	8	N	2	1.476720(7)	3	117.177(28)	4	179.615(48)
9	9	N	3	1.480007(8)	2	119.428(29)	1	175.896(49)
10	10	N	4	1.467231(9)	5	117.991(30)	6	179.848(50)
11	11	N	6	1.476320(10)	5	115.613(31)	4	177.197(51)
12	12	O	8	1.214278(11)	2	116.939(32)	3	61.362(52)
13	13	O	8	1.216425(12)	2	117.471(33)	3	-117.043(53)
14	14	O	9	1.207692(13)	3	117.447(34)	2	66.722(54)
15	15	O	9	1.213542(14)	3	116.207(35)	2	-111.979(55)
16	16	O	10	1.229370(15)	4	116.467(36)	5	-151.248(56)
17	17	O	10	1.197508(16)	4	118.170(37)	5	26.392(57)
18	18	O	11	1.204533(17)	6	117.327(38)	1	-134.095(58)
19	19	O	11	1.214875(18)	6	117.637(39)	1	48.037(59)
20	20	H	5	0.896227(19)	4	120.717(40)	3	169.875(60)
21	21	H	7	0.952914(20)	1	109.751(41)	2	-157.606(61)
22	22	H	7	0.960115(21)	1	112.638(42)	2	80.017(62)
23	23	H	7	0.959605(22)	1	105.684(43)	2	-39.439(63)

STOICHIOMETRY C7H4N4O8

SCF DONE: E(RHF) = -1078.84031213 A.U. AFTER 23 CYCLES

Alpha eigenvalues — -0.33499 -0.33329 -0.33118 -0.32700 0.09702

Estimated ionization potential: 8.91 ev

Total atomic charges:

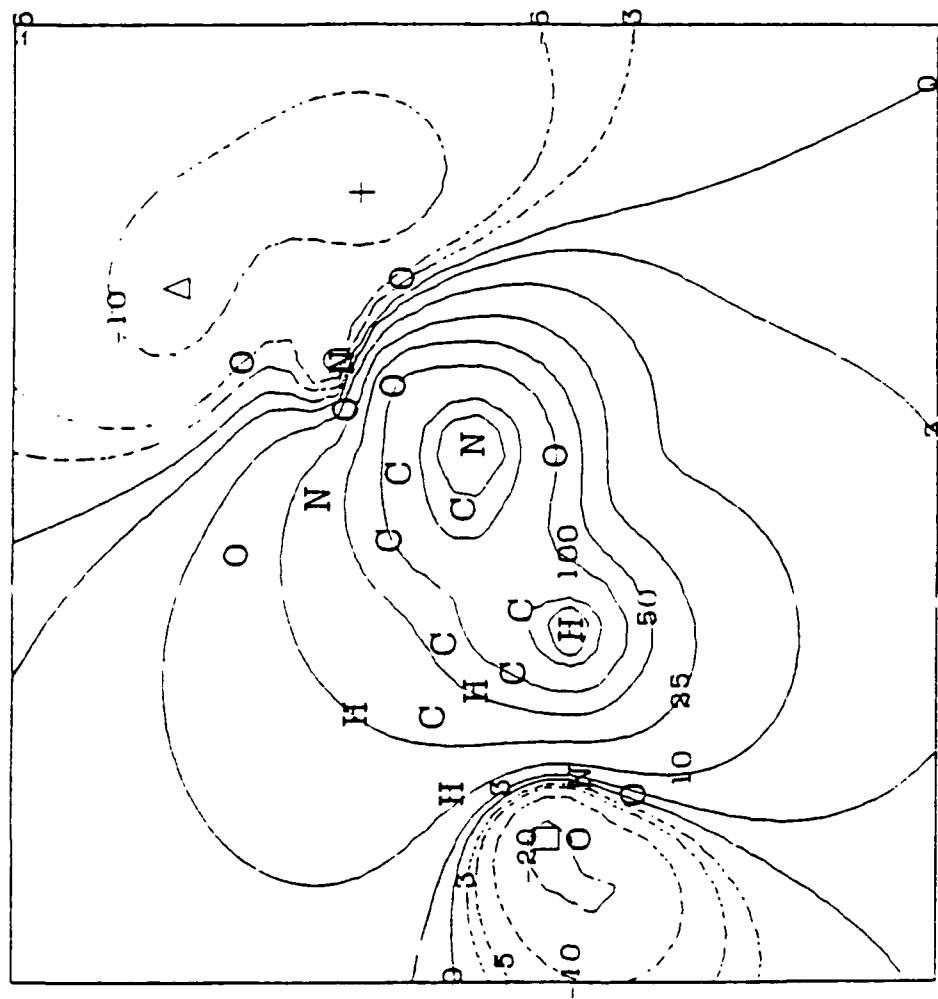
1
1 C 0.081413
2 C 0.101510
3 C 0.118168
4 C 0.116989
5 C -0.079623
6 C 0.114700
7 C -0.322111
8 N 0.176597
9 N 0.193826
10 N 0.183033
11 N 0.178602
12 O -0.176888
13 O -0.177513
14 O -0.169090
15 O -0.168483
16 O -0.185679
17 O -0.173604
18 O -0.183706
19 O -0.190938
20 H 0.150989
21 H 0.133745
22 H 0.138560
23 H 0.139503

Dipole moment (Debye): X = -3.4811 Y = -0.6377 Z = -0.1966 Tot = 3.5445

V-mid: C2-N8: 0.200
C3-N9: 0.223
C4-N10: 0.217
C6-N11: 0.211

Bond Order: C2-N8: 1.22
C3-N9: 1.21
C4-N10: 1.25
C6-N11: 1.22
N8-O12: 1.97
N8-O13: 1.96
N9-O14: 2.00
N9-O15: 1.97
N10-O16: 1.90
N10-O17: 2.05
N11-O18: 2.02
N11-O19: 1.96

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0



MINIMA

□ -23.1
○ -7.6
△ -11.8
+ -12.3

Figure SS-1. Calculated electrostatic potential, in kcal/mole, of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N9 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0

MINIMA

□ -4.8
○ -15.8
△ -5.7

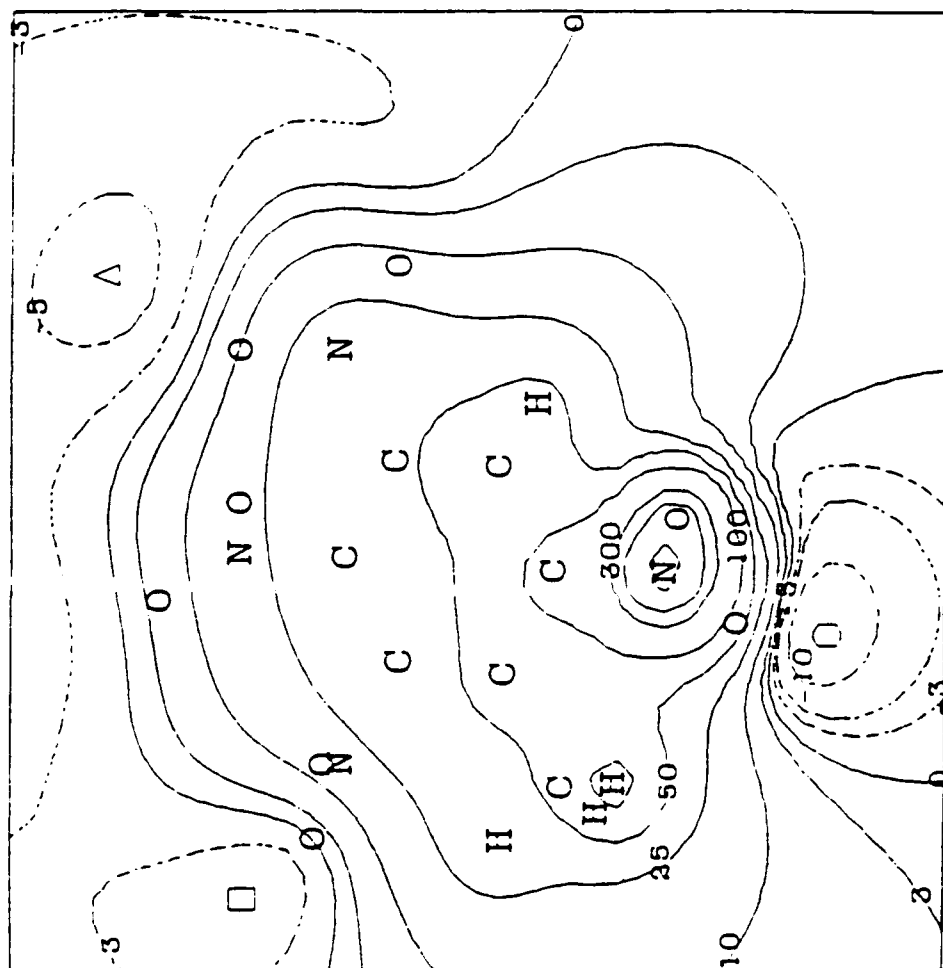
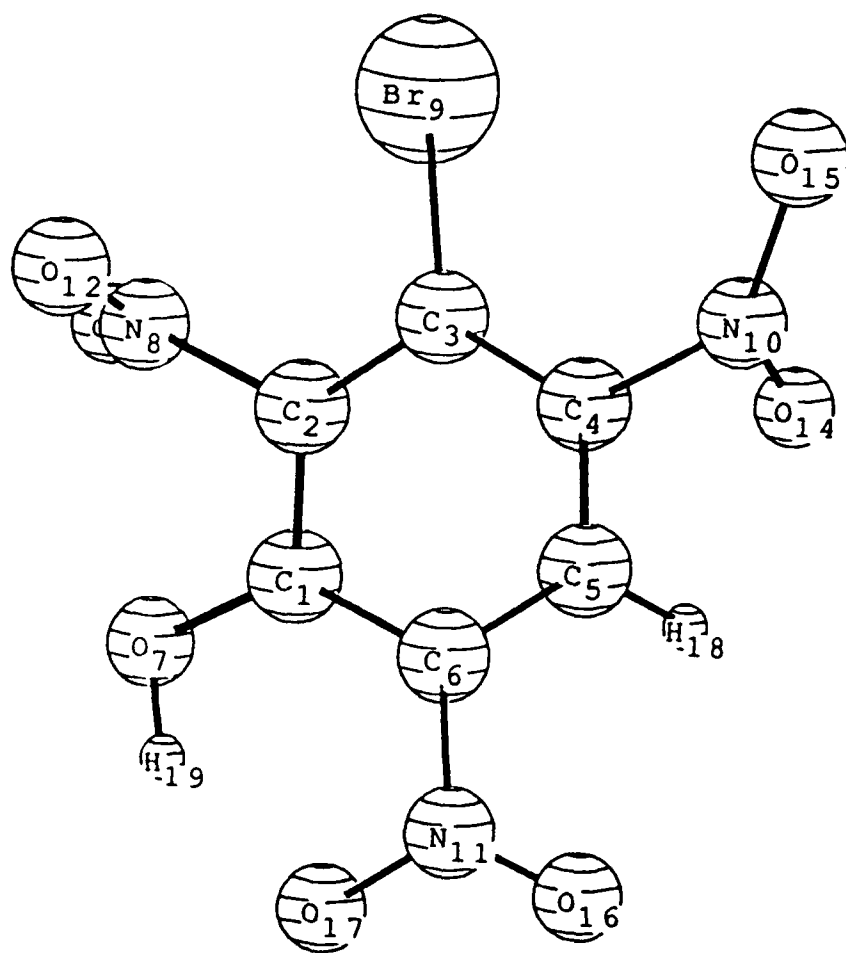


Figure SS-2. Calculated electrostatic potential, in kcal/mole, of 2,3,4,6-tetranitrotoluene, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX TT 3-BROMOPICRIC ACID

The short distances between non-bonded hydrogens and oxygens are H19-O17 (1.81 Å), H18-O16 (2.39 Å) and H18-O14 (2.46 Å)

The N10 nitro group is rotated out of the plane of the benzene ring by about 35°. The N8 nitro group is approximately perpendicular to the ring and the N11 nitro group is approximately coplanar with the ring.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
1	1	C						
2	2	C	1	1.393000(1)				
3	3	C	2	1.379119(2)	1	124.840(19)		
4	4	C	3	1.398896(3)	2	116.142(20)	1	-0.767(36)
5	5	C	4	1.370097(4)	3	121.720(21)	2	0.418(37)
6	6	C	5	1.378388(5)	4	119.955(22)	3	-0.908(38)
7	7	O	1	1.317921(6)	2	116.370(23)	3	-177.983(39)
8	8	N	2	1.479396(7)	3	119.965(24)	4	-178.983(40)
9	9	Br	3	1.871273(8)	4	125.348(25)	5	-177.755(41)
10	10	N	4	1.477524(9)	3	121.840(26)	2	-179.934(42)
11	11	N	6	1.452290(10)	5	118.380(27)	4	-178.339(43)
12	12	O	8	1.208843(11)	2	117.272(28)	3	-91.929(44)
13	13	O	8	1.209434(12)	2	116.731(29)	3	88.373(45)
14	14	O	10	1.212246(13)	4	117.269(30)	3	-146.439(46)
15	15	O	10	1.217925(14)	4	117.484(31)	3	35.977(47)
16	16	O	11	1.211311(15)	6	118.604(32)	5	3.421(48)
17	17	O	11	1.236546(16)	6	117.855(33)	5	-176.069(49)
18	18	H	5	0.960447(17)	4	120.034(34)	3	179.026(50)
19	19	H	7	0.950660(18)	1	107.542(35)	2	-178.636(51)

STOICHIOMETRY C₆H₂BrN₃O₇

SCF DONE: E(RHF) = -3470.25461235 A.U. AFTER 26 CYCLES

Alpha eigenvalues — -0.34290 -0.33656 -0.31560 -0.31353 0.10586

Estimated ionization potential 8.54 ev

Total atomic charges:

1
 1 C 0.201612
 2 C 0.071464
 3 C -0.016561
 4 C 0.080536
 5 C -0.046379
 6 C 0.053573
 7 O -0.304134
 8 N 0.186047
 9 Br 0.118185
 10 N 0.176623
 11 N 0.173891
 12 O -0.185136
 13 O -0.186380
 14 O -0.193281
 15 O -0.189150
 16 O -0.160008
 17 O -0.230146
 18 H 0.148479
 19 H 0.300765

Dipole moment (Debye):

X= -1.6305 Y= 0.3220 Z= -0.0124 Tot= 1.6620

V-mid: C2-N8: 0.184

C4-N10: 0.185

C5-N11: 0.166

Bond Order: C2-N8: 1.22

C4-N10: 1.22

C5-N11: 1.29

N8-O12: 1.99

N8-O13: 1.99

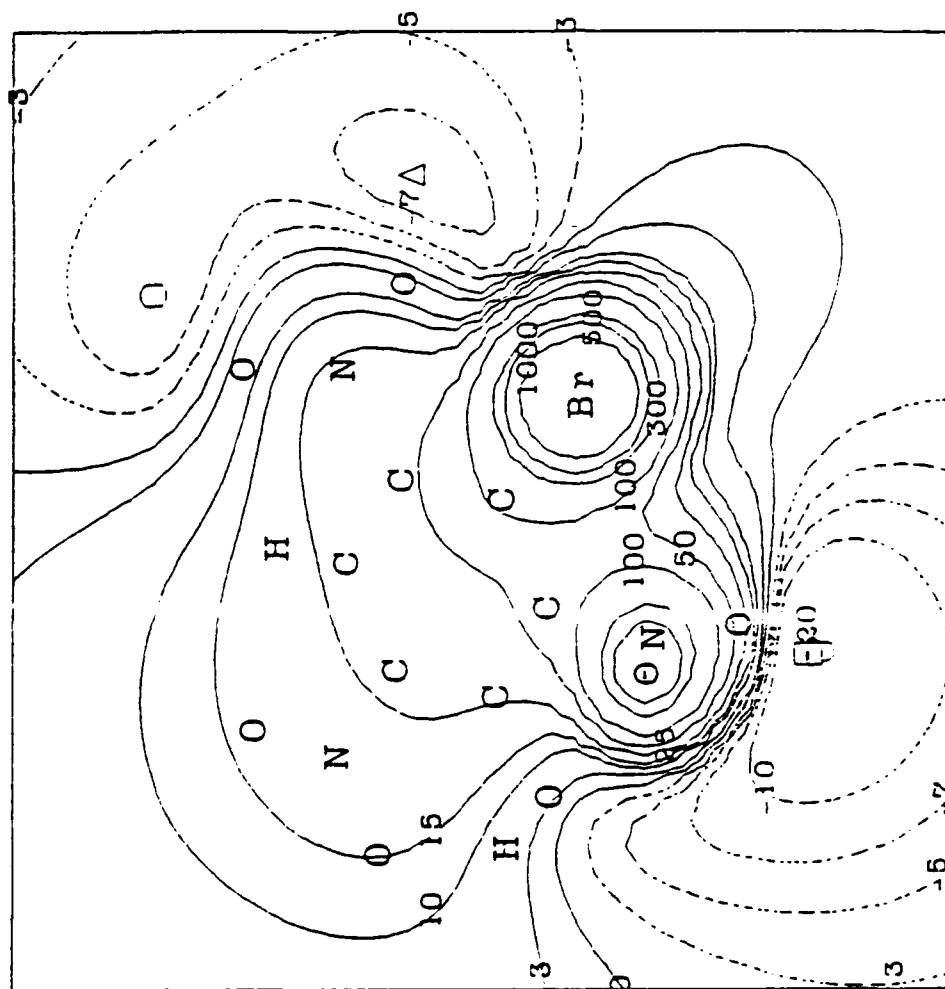
N10-O14: 1.98

N10-O15: 1.95

N11-O16: 1.98

N11-O17: 1.86

-20.0
-10.0
-7.0
-6.0
-3.0
0.0
3.0
10.0
15.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA

□ -20.4
○ -6.8
△ -8.2

Figure TT-1. Calculated electrostatic potential, in kcal/mole, of 3-bromopropionic acid, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
-1.0
0.0
3.0
10.0
25.0
30.0
35.0
40.0
45.0
50.0
100.0
300.0
500.0

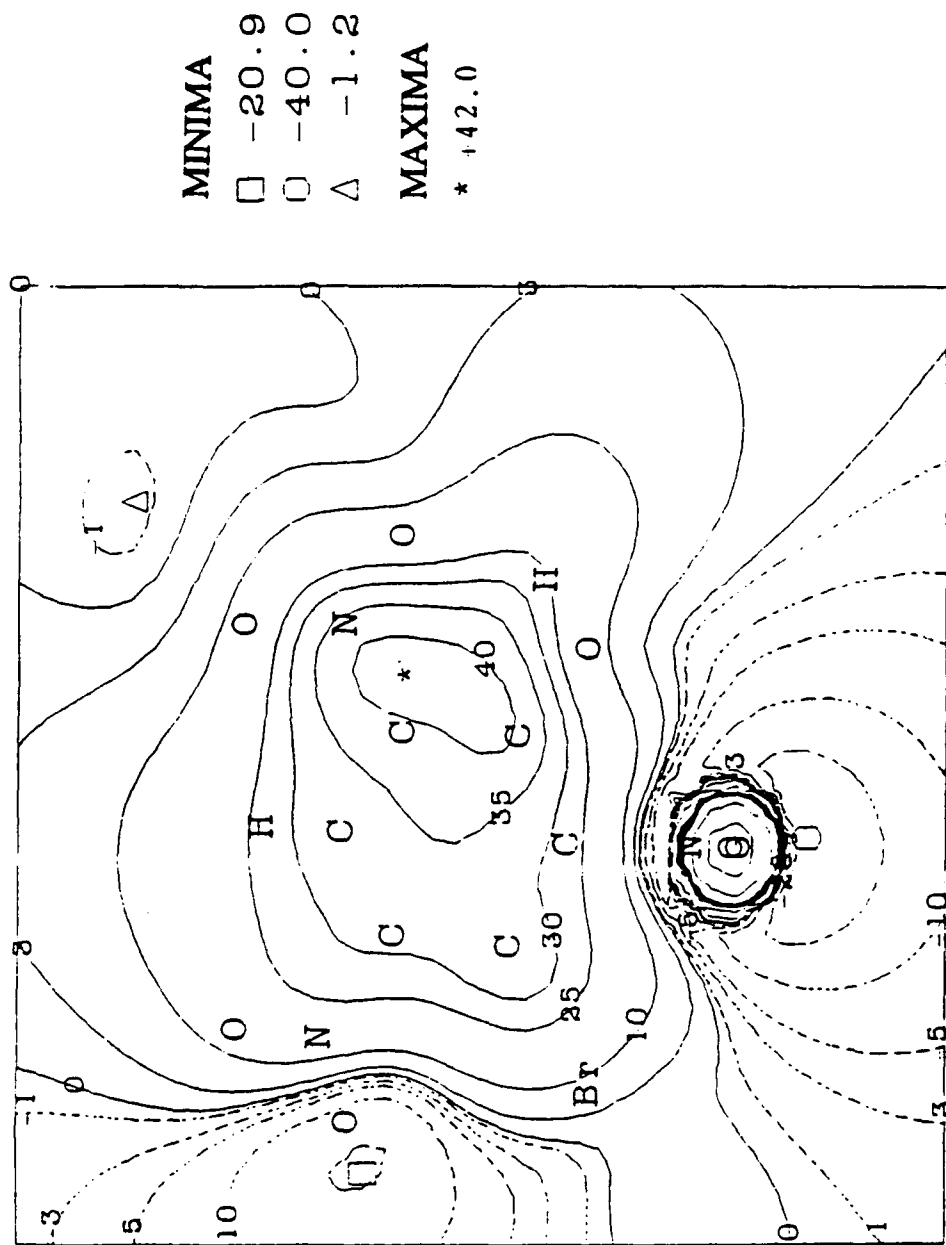
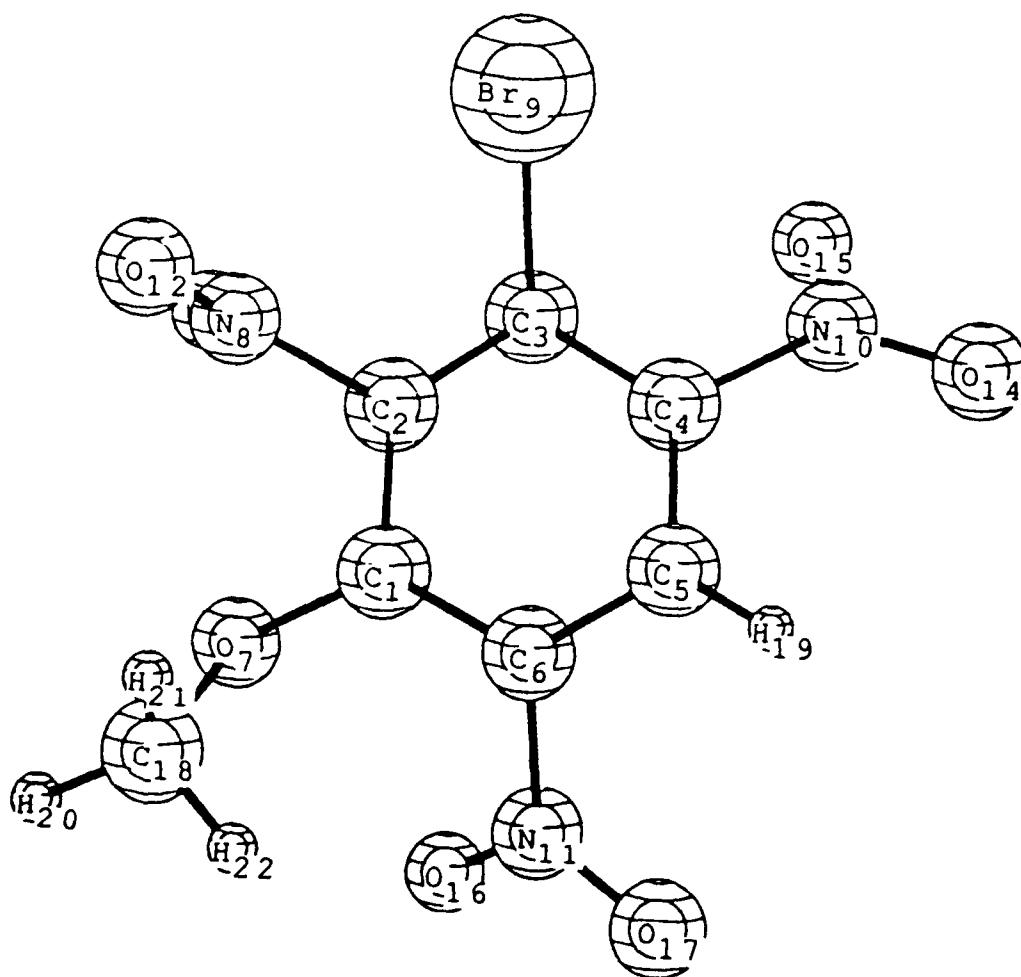


Figure TT-2. Calculated electrostatic potential, in kcal/mole, of 3-bromopicric acid, in the plane 1.75Å above the N11 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX UU
3-BROMO-2,4,6-TRINITROANISOLE

The short distances between non-bonded hydrogens and oxygens are H19-O14 (2.45 Å), H19-O17 (2.49 Å) and H22-O16 (2.47 Å)

The N8 nitro group is essentially perpendicular to the mean plane of the benzene ring, while the N10 and N11 nitro groups are both rotated by about 36°.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
J								
1	1	C						
2	2	C	1	1.379000(1)				
3	3	C	2	1.379116(2)	1	124.442(22)		
4	4	C	3	1.395400(3)	2	116.406(23)	1	-1.379(42)
5	5	C	4	1.368293(4)	3	121.775(24)	2	-1.346(43)
6	6	C	5	1.382808(5)	4	119.307(25)	3	3.569(44)
7	7	O	1	1.351355(6)	2	117.977(26)	3	-176.200(45)
8	8	N	2	1.476378(7)	3	119.163(27)	4	176.735(46)
9	9	Br	3	1.872958(8)	4	124.246(28)	5	175.728(47)
10	10	N	4	1.476587(9)	5	116.492(29)	6	-175.714(48)
11	11	N	6	1.477025(10)	5	116.722(30)	4	175.269(49)
12	12	O	8	1.201329(11)	2	117.202(31)	3	-92.123(50)
13	13	O	8	-1.200812(12)	2	116.353(32)	3	88.446(51)
14	14	O	10	1.212974(13)	4	115.902(33)	5	-35.462(52)
15	15	O	10	1.209142(14)	4	118.232(34)	5	143.432(53)
16	16	O	11	1.209457(15)	6	117.747(35)	5	-143.725(54)
17	17	O	11	1.209442(16)	6	116.999(36)	5	35.373(55)
18	18	C	7	1.398537(17)	1	117.875(37)	2	-115.577(56)
19	19	H	5	0.959648(18)	4	120.314(38)	3	-176.408(57)
20	20	H	18	0.959867(19)	7	109.535(39)	1	179.959(58)
21	21	H	18	0.960615(20)	7	109.472(40)	1	59.984(59)
22	22	H	18	0.960007(21)	7	109.495(41)	1	-59.944(60)

STOICHIOMETRY C7H4BrN3O7

SCF DONE: E(RHF) = -3509.10229704 A.U. AFTER 25 CYCLES

Alpha eigenvalues — -0.34044 -0.32306 -0.32168 -0.31901 0.11836

Estimated ionization potential: 8.69 ev

Total atomic charges:

1
 1 C 0.185275
 2 C 0.080447
 3 C -0.024495
 4 C 0.092655
 5 C -0.055062
 6 C 0.078798
 7 O -0.237359
 8 N 0.192271
 9 Br 0.111449
 10 N 0.180334
 11 N 0.179910
 12 O -0.195012
 13 O -0.180095
 14 O -0.192763
 15 O -0.185360
 16 O -0.188450
 17 O -0.193487
 18 C -0.166343
 19 H 0.145739
 20 H 0.137222
 21 H 0.117720
 22 H 0.116606

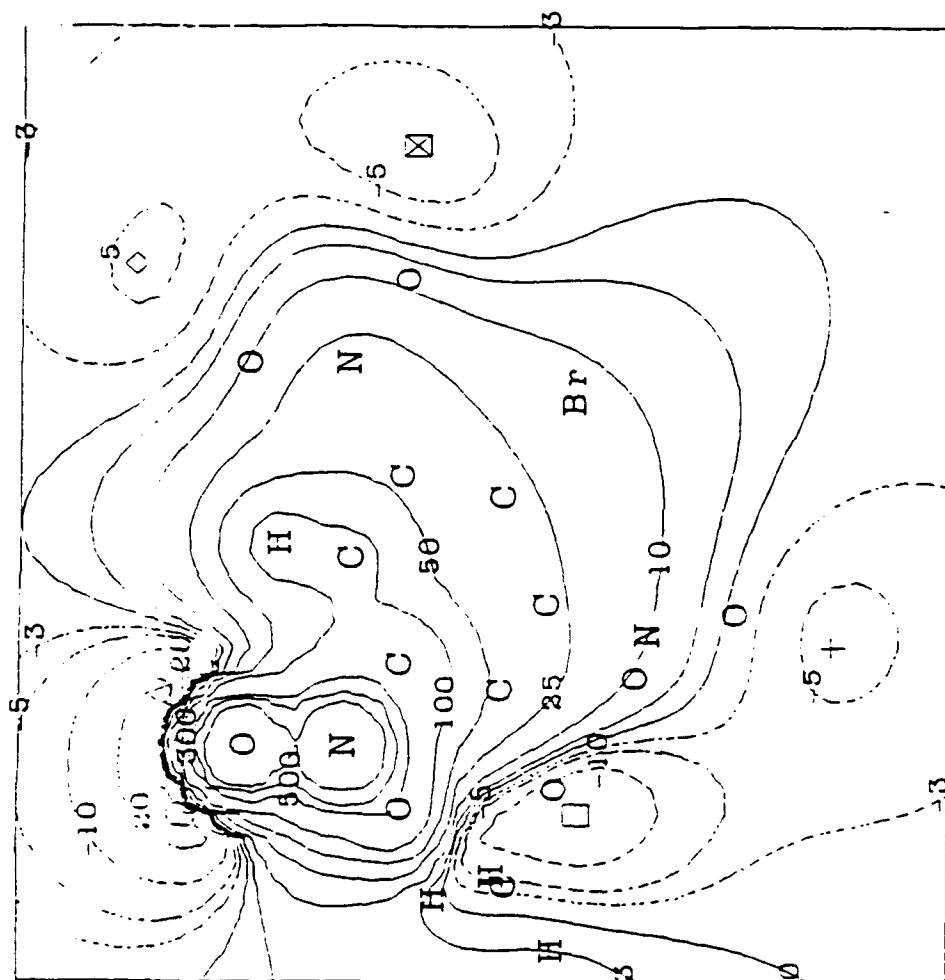
Dipole moment (Debye):

X= 1.1326 Y= -0.3745 Z= 1.3379 Tot= 1.7925

V-mid: C2-N8: 0.195
 C4-N10: 0.196
 C6-N11: 0.186

Bond Order: C2-N8: 1.22
 C4-N10: 1.22
 C6-N11: 1.22
 N8-O12: 2.03
 N8-O13: 2.03
 N10-O14: 1.97
 N10-O15: 1.99
 N11-O16: 1.99
 N11-O17: 1.99

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0



MINIMA

□ -18.4
○ -28.0
△ -24.0
+ -5.4
◇ -5.3
⊠ -6.3

Figure UU-1. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N10 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0

MINIMA

□ -4.8
○ -0.4
△ -11.6
+ -31.2
◇ -6.0
⊠ -4.7

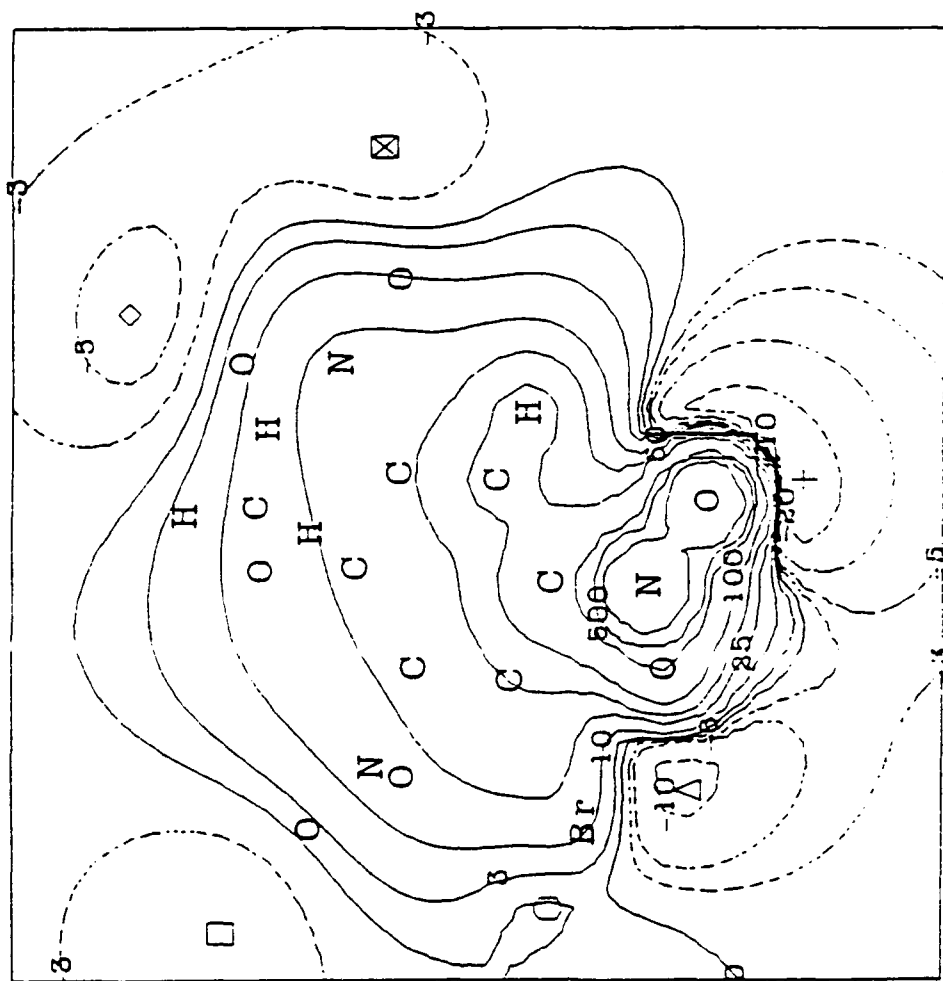
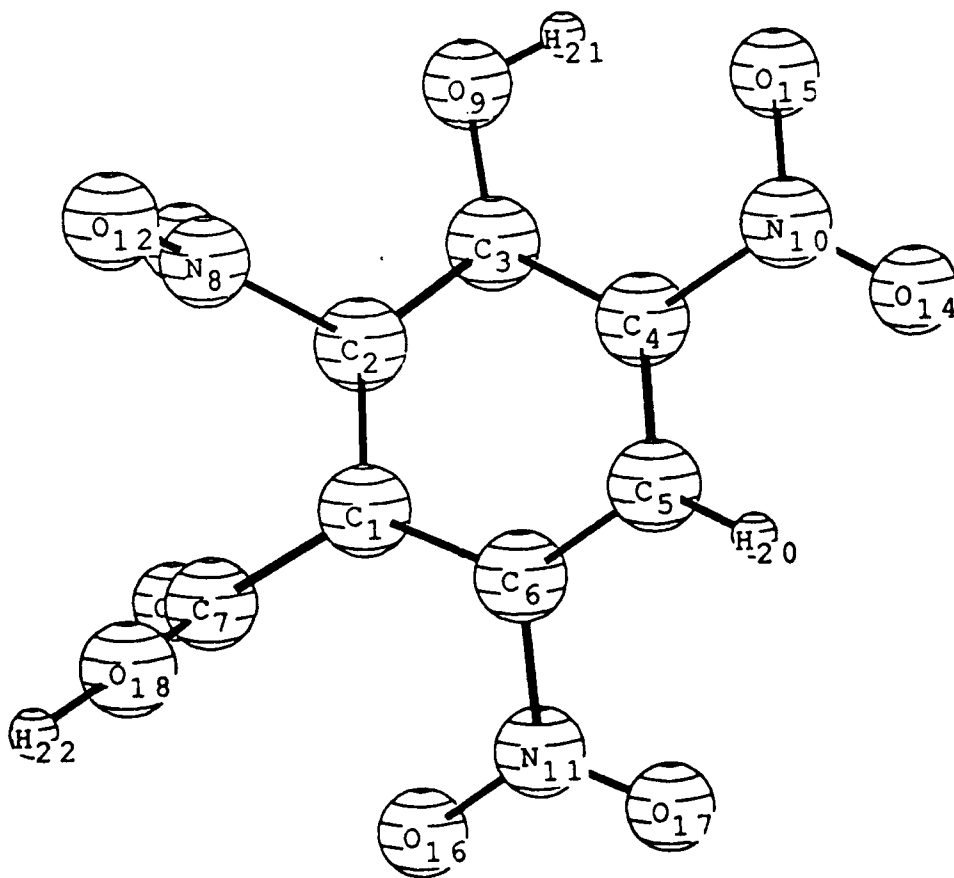


Figure UU-2. Calculated electrostatic potential, in kcal/mole, of 3-bromo-2,4,6-trinitroanisole, in the plane 1.75Å above the N11 nitro group located in the upper right corner. Projected positions of nuclei are shown. All contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

APPENDIX VV
2,4,6-TRINITRO-3-HYDROXYBENZOIC ACID

The short distances between non-bonded hydrogens and oxygens are H21-O15 (1.82 Å), H20-O14 (2.42 Å) and H20-O17 (2.38 Å)

The N8 and N11 nitro groups are rotated out of the mean plane of the benzene ring by about 85° and 15°, respectively, while the N10 nitro group is coplanar.



Z-MATRIX (ANGSTROMS AND DEGREES)								
CD	Cent	Atom	N1	Length/X	N2	Alpha/Y	N3	Beta/Z
								J
1	1	C						
2	2	C	1	1.380000(1)				
3	3	C	2	1.375419(2)	1	125.708(22)		
4	4	C	3	1.410745(3)	2	116.196(23)	1	-2.263(42) 0
5	5	C	4	1.379572(4)	3	120.865(24)	2	1.200(43) 0
6	6	C	5	1.358087(5)	4	119.608(25)	3	0.587(44) 0
7	7	C	1	1.504014(6)	2	119.832(26)	3	-176.905(45) 0
8	8	N	2	1.477542(7)	3	115.445(27)	4	175.716(46) 0
9	9	O	3	1.326100(8)	4	126.004(28)	5	179.890(47) 0
10	10	N	4	1.443422(9)	5	119.204(29)	6	-179.408(48) 0
11	11	N	6	1.478447(10)	5	117.605(30)	4	177.563(49) 0
12	12	O	8	1.206366(11)	2	116.582(31)	3	-95.761(50) 0
13	13	O	8	1.207174(12)	2	118.128(32)	3	83.498(51) 0
14	14	O	10	1.209020(13)	4	118.876(33)	5	-1.472(52) 0
15	15	O	10	1.232903(14)	4	118.891(34)	5	-179.861(53) 0
16	16	O	11	1.218424(15)	6	117.372(35)	5	-165.606(54) 0
17	17	O	11	1.224370(16)	6	117.658(36)	5	15.063(55) 0
18	18	O	7	1.276162(17)	1	114.312(37)	2	-98.637(56) 0
19	19	O	7	1.232137(18)	1	119.602(38)	2	74.313(57) 0
20	20	H	5	0.938906(19)	4	120.737(39)	3	179.296(58) 0
21	21	H	9	0.898851(20)	3	107.772(40)	4	5.968(59) 0
22	22	H	18	0.875728(21)	7	120.356(41)	1	-177.756(60) 0

STOICHIOMETRY C7H3N3O9

SCF DONE: E(RHF) = -1098.71997240

Alpha eigenvalues — -0.34245 -0.33877 -0.31967 -0.31152 0.10020

Estimated ionization potential: 8.48 ev

Total atomic charges:

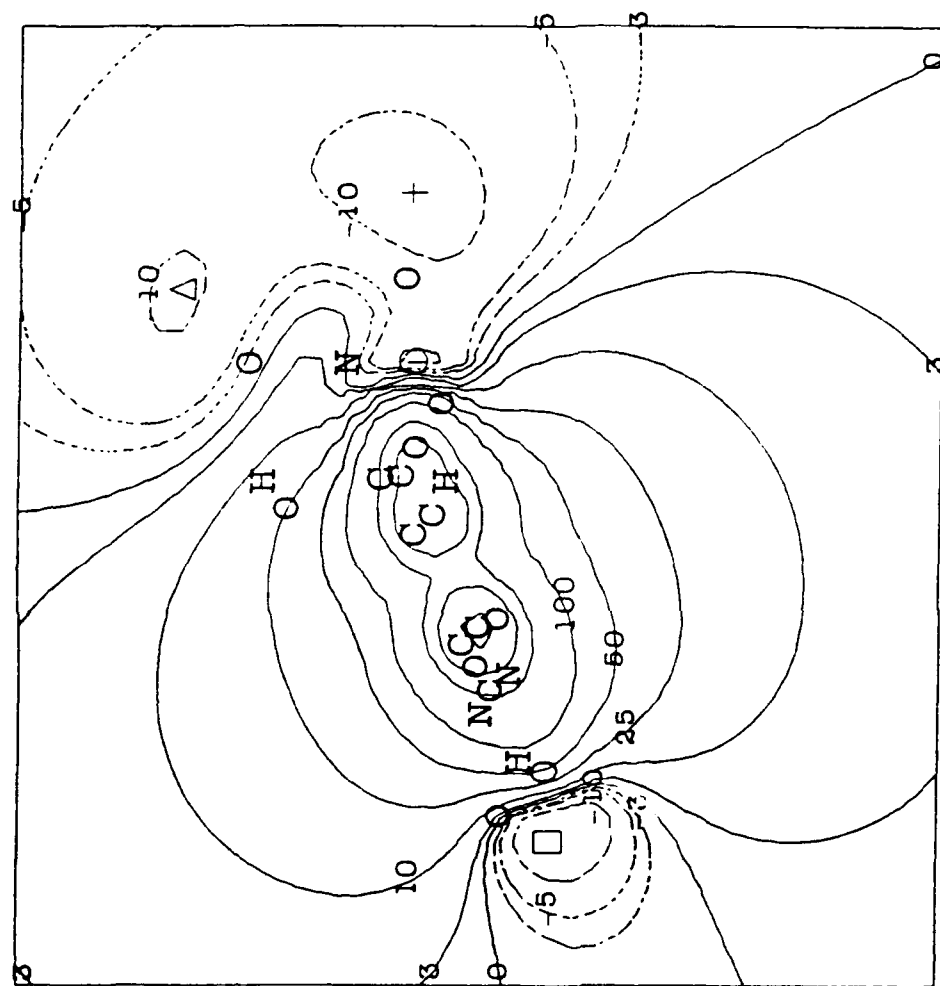
1
 1 C 0.042209
 2 C 0.078744
 3 C 0.200410
 4 C 0.062703
 5 C -0.058925
 6 C 0.089312
 7 C 0.380530
 8 N 0.185185
 9 O -0.324553
 10 N 0.172504
 11 N 0.174672
 12 O -0.192965
 13 O -0.180343
 14 O -0.161448
 15 O -0.229640
 16 O -0.197011
 17 O -0.189305
 18 O -0.374100
 19 O -0.257961
 20 H 0.153092
 21 H 0.314924
 22 H 0.311966

Dipole moment (Debye):

X= -0.4087 Y= 0.7248 Z= 0.9239 Tot= 1.2434

Bond Order: C2-N8: 1.22 V-mid: C2-N8: 0.189
 C4-N10: 1.31 C4-N10: 0.173
 C6-N11: 1.22 C6-N11: 0.189
 N8-O12: 2.01
 N8-O13: 2.00
 N10-O14: 1.99
 N10-O15: 1.88
 N11-O16: 1.95
 N11-O17: 1.92

-10.0
-5.0
-3.0
0.0
3.0
10.0
25.0
50.0
100.0
300.0
500.0
1000.0

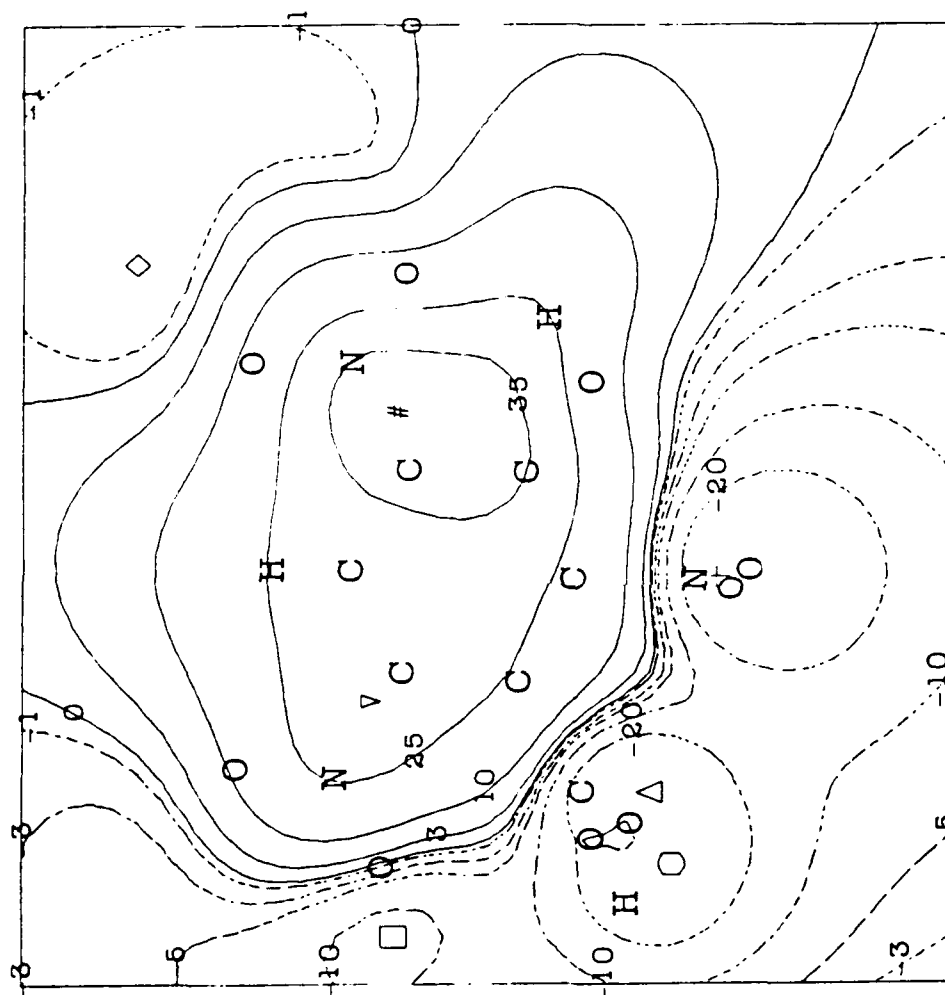


MINIMA

- -18.1
- -11.1
- △ -10.5
- + -12.3

Figure VV-1. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N8 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

-20.0
-10.0
-5.0
-3.0
-1.0
0.0
3.0
10.0
25.0
35.0



MINIMA	
□	-11.7
○	-42.0
△	-39.4
+	-38.0
◇	-2.4
MAXIMA	
▽	+32.0
#	+40.7

Figure VV-2. Calculated electrostatic potential, in kcal/mole, of 2,4,6-trinitro-3-hydroxybenzoic acid, in the plane 1.75Å above the N10 nitro group located in the upper right corner. The zero contours are indicated. Dashed contours represent negative potentials; the magnitudes of all contours are listed at the left of the figure. The positions of planar minima and maxima are indicated; their values are given at the right of the figure.

REFERENCES

1. J. H. Bryden, *Acta Cryst.* **B28**, 1395 (1972).
2. Richard Gilardi, Cliff George and Judith Flippen-Anderson, X-ray Crystallography of Polysubstituted Nitrobenzenes - Progress Report No. 2, Naval Research Laboratory, (1988).
3. Richard Gilardi, Cliff George and Judith Flippen-Anderson, X-ray Crystallography of Polysubstituted Nitrobenzenes - Progress Report No. 3, Naval Research Laboratory, (1988).
4. Richard Gilardi, Cliff George and Judith Flippen-Anderson, X-ray Crystallography of Polysubstituted Nitrobenzenes - Progress Report No. 1, Naval Research Laboratory, (1988).
5. J. R. Holden, C. Dickinson, *J. Phys. Chem.* **71**, 1127 (1967).
6. Richard Gilardi, Naval Research Laboratory, Washington, D.C.
7. M. A. Pierce-Butler, *Acta Cryst.* **B38**, 3097 (1982).
8. S. K. Bhattacharjee and H. L. Ammon, *Acta Cryst.* **B37**, 2082 (1981).
9. A. L. Rheingold, Personal communications.
10. C. Dickinson, J. M. Stewart, J. R. Holden, *Acta Cryst.* **B21**, 663 (1966).
11. H. H. Cady and A. C. Larson, *Acta Cryst.* **B18**, 485 (1965).
12. J. R. Holden, *Acta Cryst.* **B22**, 545 (1967).
13. P. Politzer and S. Ranganathan, *Chem. Phys. Lett.* **124**, 527 (1986).
14. J. Sharma and F. J. Owens, *Chem. Phys. Lett.* **61**, (1979) 280.
15. J. Sharma, W. L. Garrett, F. J. Owens and V. L. Vogel, *J. Phys. Chem.* **86**, (1982) 1657.
16. F. J. Owens, *J. Mol. Struct. (THEOCHEM)* **121**, (1985) 213.
17. F. J. Owens, K. Jayasuriya, L. Abrahmsen and P. Politzer, *Chem. Phys. Lett.* **116**, (1985) 434.
18. F. J. Owens and J. Sharma, *J. Appl. Phys.* **51**, (1985) 1494.
19. A. C. Gonzalez, C. W. Larson, D. F. McMillen and D. M. Golden, *J. Phys. Chem.* **89**, (1985) 4809.
20. R. S. Mulliken, *J. Chem. Phys.* **23**, (1955) 1833.
21. S. Fliszar, *J. Am. Chem. Soc.* **102**, (1980) 6946.
22. S. Fliszar, "Charge Distributions and Chemical Effects", Springer-Verlag, Heidelberg, New York, 1983.

23. R. Gilardi, C. George and J. Flippen-Anderson, Naval Research Laboratory, Washington, D.C.
24. J. S. Willis, J. H. Stewart, H. L. Ammon, H. S. Preston, R. E. Gilyab and P. M. Harris, *Acta Cryst.* **B27**, 786 (1971).
25. E. N. Duesler, J. H. Engelmann, D. Y. Curtin and I. C. Paul, *Cryst. Struct. Commun.* **7** (1978) 449.
26. C. S. Choi and J. E. Abel, *Acta Cryst.* **B28**, 193 (1972).
27. A. L. Rheingold, Department of Chemistry, University of Delaware.
28. W. R. Carper, L. P. Davis and M. W. Extine, *J. Phys. Chem.* **86**, 469 (1982).
29. J. R. Holden, C. Dickinson and C. M. Bock, *J. Phys. Chem.* **76**, 3597 (1972).
30. C.M. Gramaccioli, R. Destro and M. Simonetta, *Acta Cryst.* **B24**, 129 (1968).
31. J. C. Barnes, J. A. Chudek, R. Foster, F. Jarrett, F. Mackie, J. Paton and D. R. Twiselton, *Tetrahedron*, **40**, 1595 (1984).
32. M. J. Kamlet and H. G. Adolph, *Propellants Explosives Pyrotech.* **4**, (1979) 30.
33. B. W. Dodson and R. A. Graham, in "Shock Waves in Condensed Materials" W. J. Nellis, L. Seaman and R. A. Graham (Eds.), (American Institute of Physics, New York, 1982).
34. P. Politzer, J. M. Seminario and P. R. Bolduc, *Chem. Phys. Lett.* **158**, (1989) 463.
35. R. C. Weast, Ed., "Handbook of Chemistry and Physics", 49th Ed. (Chemical Rubber Co., Cleveland, 1968) p. D-91.
36. L. Pauling, "The Nature of the Chemical Bond", 3rd Ed. (Cornell University Press, Ithaca, 1960) section 12-6.
37. A. T. Nielsen, in "The Chemistry of the Nitro and Nitroso Groups", Part 1, H. Feuer, Ed. (Interscience, New York, 1969), Ch. 7.
38. J. S. Murray, P. Lane, P. Politzer, P. R. Bolduc and R. L. McKenney, Jr., *J. Mol. Struct. (THEOCHEM)*, in press.
39. S. Iyer, *Propellants Explosives Pyrotech.* **7**, (1982) 37.
40. Air Force impact sensitivity data received from Eglin AFB.
41. D. Weinstein and F. J. Owens, unpublished data.
42. R. N. Rogers, *Anal. Chem.* **39**, (1967) 731.
43. J. C. Dacons, H. G. Adolph and M. J. Kamlet, *J. Phys. Chem.* **74**, (1970) 3035.
44. S. A. Shackelford, J. W. Beckmann and J. S. Wilkes, *J. Org. Chem.* **42**, (1977) 4201.

45. S. Bulusu and T. Axenrod, *Organic Mass Spectrom.* **14**, (1979) 585.
46. R. N. Rogers, J. L. Janney and M. H. Ebinger, *Thermochim. Acta* **59**, (1982) 287.
47. S. Bulusu and J. R. Autera, *J. Energetic Materials*, **133**, June 1983.
48. J. Sharma, J. C. Hoffsomer, D. J. Glover, C. S. Coffey, F. Santiago, A. Stolovy and S. Yasuda, in *Shock Waves in Condensed Matter*, J. R. Assay, R. A. Graham and G. K. Straub, eds., Elsevier, 1983, pp. 543-546.
49. W. Tsang, D. Robaugh and W. G. Mallard, *J. Phys. Chem.* **90**, (1986) 5968.
50. J. Sharma, J. W. Forbes, C. S. Coffey and T. P. Liddiard, *J. Phys. Chem.* **91**, (1987) 5139.
51. W. M. Trott and A. M. Renlund, *J. Phys. Chem.* **92**, (1988) 5921.
52. C. B. Storm, J. R. Stine and J. F. Kramer, *Proc. NATO Advanced Study Institute on Chemistry and Physics of Molecular Processes in Energetic Materials, Sicily, September, 1989*, in press.
53. P. R. Bolduc and S. A. Obert, private communication.
54. R. Gilardi, personal communication.
55. M. J. Kamlet, J. C. Hoffsomer and H. G. Adoph, *J. Amer. Chem. Soc.* **84**, 3925 (1962).